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AN OVERVIEW OF THE BOLTZMANN TRANSPORT EQUATION SOLUTION FOR NEUTRONS, PHOTONS AND ELECTRONS IN CARTESIAN GEOMETRY

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ABSTRACT

Questions regarding accuracy and efficiency of deterministic transport methods are still on our mind today, even with modern supercomputers. The most versatile and widely used deterministic methods are the P_N approximation, the S_N method (discrete ordinates method) and their variants. In the discrete ordinates (S_N) formulations of the transport equation, it is assumed that the linearized Boltzmann equation only holds for a set of distinct numerical values of the direction-of-motion variables. In this work, looking forward to confirm the capabilities of deterministic methods in obtaining accurate results, we present a general overview of deterministic methods to solve the Boltzmann transport equation for neutral and charged particles. First, we describe a review in the Laplace transform technique applied to S_N two dimensional transport equation in a rectangular domain considering Compton scattering. Next, we solved the Fokker-Planck (FP) equation, an alternative approach for the Boltzmann transport equation, assuming a monoenergetic electron beam in a rectangular domain. The main idea relies on applying the P_N approximation, a recent advance in the class of deterministic methods, in the angular variable, to the two dimensional Fokker-Planck equation and then applying the Laplace Transform in the spatial x-variable. Numerical results are given to illustrate the accuracy of deterministic methods presented.

1. INTRODUCTION

The Boltzmann equation is an integro-differential equation representing a wide range of transport problems from astrophysics to traffic low [1]. Elegant analytical and numerical techniques have been developed to solve the Boltzmann equation for a broad class of transport and radiative transfer problems. These methods follow two distinct schools of thought: the probabilistic school, such as the Monte Carlo methods, which basic philosophy is to solve approximately the exact problem, and the deterministic school, such as the discrete ordinates methods, which basic philosophy is to solve exactly an approximate problem. The stochastic Monte Carlo method often is considered to be the ultimate numerical approach for radiation transport calculations, especially for complicated geometries. However if differential distributions are required, then a deterministic solution of the Boltzmann transport equation is often more efficient.

Questions regarding accuracy and efficiency of deterministic transport methods are still on our mind today, even with modern supercomputers. The most versatile and widely used deterministic methods are the P_N approximation [2, 3], the S_N method (discrete ordinates method) [4, 5] and their variants [6, 7]. In the discrete ordinates (S_N) formulations of the transport equation, it is assumed that the linearized Boltzmann equation only holds for a set of distinct numerical values of the direction-of-motion variables.

In the last decade, the LTS_N method was presented in the literature. This method solves, analytically, the discrete ordinates equation (S_N equation) in a slab by the Laplace transform technique. The main idea comprehends the following steps: application of the Laplace transform technique to the set of the S_N equations, solution of the resulting algebraic equation by the matrix diagonalization approach and inversion of the transformed angular flux by standard results of the Laplace transform theory. In earlier works [6, 8] the LTS_N method was applied in the solution of two dimensional transport equation assuming neutrons and photons in cartesian geometry.

On the other hand, in a recent work [9] we solved the Fokker-Planck (FP) equation, an alternative approach for the Boltzmann transport equation, assuming a monoenergetic electron beam in a rectangular domain. The Fokker-Planck (FP) approximation represents the impact of soft reactions as continuously slowing down the electrons, while also continuously changing their direction; e.g., a monodirectional beam will be dispersed into a finite beam width. This approximation can be derived from a Taylor series expansion of the integrand in the scatter source term appearing in the Boltzmann equation, with the assumption that only small changes in energy and direction are significant. The main idea relies on applying the P_N approximation, a recent advance in the class of deterministic methods, in the angular variable, to the two dimensional Fokker-Planck equation and then applying the Laplace Transform in the spatial x-variable. As a result, a first order linear differential equation in the spatial y-variable, is attained, which the solution is straightforward. The P_N approximation consists in expanding the angular variable of the angular flux in terms of the Legendre polynomials. Therefore, in this work, looking forward to confirm the capabilities of deterministic methods in obtaining accurate results, we present a general overview of deterministic methods to solve the Boltzmann transport equation for neutral and charged particles. Indeed, to reach our objectives, we organized this work as follows: in section 2 we present a review in the Laplace transform technique applied to S_N two dimensional transport equation in a rectangular domain considering Compton scattering. In section 3 we describe in detail the two dimensional Fokker-Planck (FP) equation solution. In section 4 we report numerical simulations and comparisons. Concluding remarks and suggestions for future work are given in section 5.

2. THE LTS_N NODAL SOLUTION IN A RECTANGULAR DOMAIN

Let us consider the two dimensional S_N nodal problem assuming Klein-Nishina scattering kernel and multigroup model [8]:

$$\mu_n \frac{\partial}{\partial x} I_{jn}(x,y) + \eta_n \frac{\partial}{\partial y} I_{jn}(x,y) + \mu_{lj} I_{jn}(x,y) =$$

$$= \frac{\Delta}{3} \sum_{l=0}^{L} \frac{2l+1}{2} \sum_{r=1}^{G} c_r \alpha k_{rj} P_l (1 + \lambda_r - \lambda_j) P_l(\mu_n) \sum_{i=1}^{N} P_l(\mu_i) I_{ri}(x,y) \omega_i, \qquad (1)$$

subject to vacuum boundary condition in a rectangle $0 \leq x \leq a$ and $0 \leq y \leq b$. Here $j = 1 : G$, $n = 1 : N$, $N = \frac{M(M+2)}{2}$ is the cardinality of the discrete ordinates set (number of discrete directions), M represents the order of the angular quadrature, G is the number of energy groups (wavelengths), μ_{lj} is the linear attenuation coefficient, $I_{jn}(x, y) = I(x, y, \lambda_j, \Omega_n)$ is the angular flux at the discrete direction $\Omega_n = (\mu_n, \eta_n)$ for the j_{th} group, ω_i are the Level Symetric Quadrature (LQ_N) weights and $k_{rj} = k(\lambda_r, \lambda_j)$ is the Klein-Nishina scattering kernel [6, 10].

It is important to mention that, in this work, the integral term in the wavelenght variable is approximated by the Simpson's rule [10].

To construct the LTS_N nodal solution for problem (1) we begin performing the transverse integration of this equation. This procedure yields to the set of the ensuing two coupled S_N equations,

$$\eta_n \frac{\partial}{\partial y} I_{jny}(y) + \frac{\mu_n}{a}\Big[I_{jn}(a, y) - I_{jn}(0, y)\Big] + \mu_{lj} I_{jny}(y) =$$
$$= \frac{\Delta}{3} \sum_{l=0}^{L} \frac{2l+1}{2} \sum_{r=1}^{G} c_r \alpha k_{rj} P_l(1 + \lambda_r - \lambda_j) P_l(\mu_n) \sum_{i=1}^{N} P_l(\mu_i) I_{riy}(y) \omega_i, \tag{2}$$

for $j = 1 : G$, $n = 1 : N$. Here $I_{jn}(a, y)$ and $I_{jn}(0, y)$ are the angular fluxes exiting at the boundary and the average angular flux is written like,

$$I_{jny}(y) = \frac{1}{a} \int_0^a I_{jn}(x, y) dx. \tag{3}$$

$$\mu_n \frac{\partial}{\partial x} I_{jnx}(x) + \frac{\eta_n}{b}\Big[I_{jn}(x, 0) - I_{jn}(x, b)\Big] + \mu_{lj} I_{jnx}(x) =$$
$$= \frac{\Delta}{3} \sum_{l=0}^{L} \frac{2l+1}{2} \sum_{r=1}^{G} c_r \alpha k_{rj} P_l(1 + \lambda_r - \lambda_j) P_l(\mu_n) \sum_{i=1}^{N} P_l(\mu_i) I_{rix}(x) \omega_i, \tag{4}$$

for $j = 1 : G$, $n = 1 : N$. Here $I_{jn}(x, b)$ and $I_{jn}(x, 0)$ are the angular fluxes exiting at the boundary and the average angular flux is written like,

$$I_{jnx}(x) = \frac{1}{b} \int_0^b I_{jn}(x, y) dy. \tag{5}$$

To this point we are in position to apply the LTS_N method. Indeed, we begin applying the Laplace transform technique in equation (2). This procedure yields:

$$s\overline{I_{jny}}(s) + \frac{\mu_{lj}}{\eta_n}\overline{I_{jny}}(s) - \frac{\Delta}{3\eta_n} \sum_{l=0}^{L} \frac{2l+1}{2} \sum_{r=1}^{G} c_r \alpha k_{rj} P_l(1 + \lambda_r - \lambda_j) P_l(\mu_n) \times$$
$$\times \sum_{i=1}^{N} P_l(\mu_i) \overline{I_{riy}}(s) \omega_i = I_{jny}(0) - \frac{\mu_n}{a\eta_n}\Big[\overline{I_{jn}}(a, s) - \overline{I_{jn}}(0, s)\Big], \tag{6}$$

for $j = 1 : G$ and $n = 1 : N$, which can be recast in matrix form like,

$$(sI - B_{jny})\overline{I_{jny}}(s) = I_{jny}(0) + \overline{Z_{(j-1)y}}(s) + \overline{S_{jny}}(s). \tag{7}$$

Here $\overline{I_{jny}}(s)$ is the N components of the angular flux Laplace transformed vector in y variable and $I_{jny}(0)$ is the N components of the angular flux vector in y variable at y = 0. They have the form:

$$\overline{I_{jny}}(s) = \left[\overline{I_{j1y}}(s) \quad \overline{I_{j2y}}(s) \quad ... \quad \overline{I_{jNy}}(s)\right]^T, \tag{8}$$

$$I_{jny}(0) = \left[I_{j1y}(0) \quad I_{j2y}(0) \quad ... \quad I_{jNy}(0)\right]^T. \tag{9}$$

On the other hand, the components of matrix B_{jny} are given by,

$$b_y(p,q) = \begin{cases} -\frac{\mu_{lj}}{\eta_p} + \frac{\Delta}{3\eta_p}\sum_{l=0}^{L}\frac{2l+1}{2}c_j\alpha k_{jj}P_l(\mu_p)P_l(\mu_p)\omega_q & \text{se } p = q \\ \frac{\Delta}{3\eta_p}\sum_{l=0}^{L}\frac{2l+1}{2}c_j\alpha k_{jj}P_l(\mu_p)P_l(\mu_q)\omega_q & \text{se } p \neq q \end{cases} \tag{10}$$

and the scattering term reads like,

$$\overline{Z_{(j-1)y}}(s) = \sum_{i=1}^{j-1} H_{iy}\overline{I_{iny}}(s), \tag{11}$$

where the entries of constant matrix H_{iy} are written like,

$$h_y(p,q) = \begin{cases} \frac{\Delta}{3\eta_p}\sum_{l=0}^{L}\frac{2l+1}{2}c_i\alpha k_{ij}P_l(1+\lambda_i-\lambda_j)P_l(\mu_p)P_l(\mu_p)\omega_q & \text{se } p = q \\ -\frac{\Delta}{3\eta_p}\sum_{l=0}^{L}\frac{2l+1}{2}c_i\alpha k_{ij}P_l(1+\lambda_i-\lambda_j)P_l(\mu_p)P_l(\mu_q)\omega_q & \text{se } p \neq q. \end{cases} \tag{12}$$

The vector $\overline{S_{jny}}(s)$ has the generic component:

$$\overline{S_{jiy}}(s) = -\frac{\mu_i}{a\eta_i}\Big[\overline{I_{ji}}(a,s) - \overline{I_{ji}}(0,s)\Big]. \tag{13}$$

Similar procedure in the x variable leads to the ensuing linear algebraic system,

$$s\overline{I_{jnx}}(s) + \frac{\mu_{lj}}{\mu_n}\overline{I_{jnx}}(s) - \frac{\Delta}{3\mu_n}\sum_{l=0}^{L}\frac{2l+1}{2}\sum_{r=1}^{G}c_r\alpha k_{rj}P_l(1+\lambda_r-\lambda_j)P_l(\mu_n) \times$$
$$\times\sum_{i=1}^{N}P_l(\mu_i)\overline{I_{rix}}(s)\omega_i = I_{jnx}(0) - \frac{\eta_n}{b\mu_n}\Big[\overline{I_{jn}}(s,b) - \overline{I_{jn}}(s,0)\Big], \tag{14}$$

which again can be recast in the matrix form as,

$$(sI - A_{jnx})\overline{I_{jnx}}(s) = I_{jnx}(0) + \overline{Z_{(j-1)x}}(s) + \overline{S_{jnx}}(s). \tag{15}$$

Here $\overline{I_{jnx}(s)}$ is the N components of the angular flux Laplace transformed vector in x variable and $I_{jnx}(0)$ is the N components of the angular flux vector in x variable at x = 0. They have the form:

$$\overline{I_{jnx}(s)} = \left[\overline{I_{j1x}(s)} \quad \overline{I_{j2x}(s)} \quad ... \quad \overline{I_{jNx}(s)}\right]^T, \tag{16}$$

$$I_{jnx}(0) = \left[I_{j1x}(0) \quad I_{j2x}(0) \quad ... \quad I_{jNx}(0)\right]^T. \tag{17}$$

Bearing in mind that for the Klein-Nishina scattering kernel the wavelength ranges from λ_0 to $\lambda_0 + 2$ (λ_0 is the wavelength of the slab incoming radiation), we discretize, without loss of generality, this interval in five sub-intervals, we mean five groups, with the main feature that the first group (group 1) corresponds to the sub-interval with shortest wavelength and higher energy and group 5, to the sub-interval with the longest wavelength and lowest energy.

Solving recursively equations (7) and (15) for increasing wavelength, (j from 1 to 5) due to the down-scattering, the LTS$_N$ solution for these equations are given by

$$\overline{I_{jny}}(s) = (sI - B_{jny})^{-1}[I_{jny}(0) + \overline{Z_{(j-1)y}}(s) + \overline{S_{jny}}(s)] \tag{18}$$

and

$$\overline{I_{jnx}}(s) = (sI - A_{jnx})^{-1}[I_{jnx}(0) + \overline{Z_{(j-1)x}}(s) + \overline{S_{jnx}}(s)]. \tag{19}$$

Taking the Laplace inversion of the above ansatz we get,

$$I_{jny}(y) = \mathcal{L}^{-1}\{(sI - B_{jny})^{-1}[I_{jny}(0) + \overline{Z_{(j-1)y}}(s) + \overline{S_{jny}}(s)]\} \tag{20}$$

and

$$I_{jnx}(x) = \mathcal{L}^{-1}\{(sI - A_{jnx})^{-1}[I_{jnx}(0) + \overline{Z_{(j-1)x}}(s) + \overline{S_{jnx}}(s)]\}, \tag{21}$$

which by the Heaviside expansion technique can be recast like [10],

$$I_{jny}(y) = \sum_{k=1}^{jn} \beta_k e^{s_k y} I_{jny}(0) + Z_{(j-1)y}(y) * \mathcal{L}^{-1}\{(sI - B_{jny})^{-1}\} + \\ + S_{jny}(y) * \mathcal{L}^{-1}\{(sI - B_{jny})^{-1}\} \tag{22}$$

and

$$I_{jnx}(x) = \sum_{k=1}^{jn} \beta_k e^{s_k x} I_{jnx}(0) + Z_{(j-1)x}(x) * \mathcal{L}^{-1}\{(sI - A_{jnx})^{-1}\} + \\ + S_{jnx}(x) * \mathcal{L}^{-1}\{(sI - A_{jnx})^{-1}\} \tag{23}$$

Here star denotes convolution. To complete the solution we have to determine the unknown leakage angular fluxes at boundary namely $I_{jn}(x, 0)$, $I_{jn}(0, y)$, $I_{jn}(x, b)$ and $I_{jn}(a, y)$. Following the work of Hauser [8] which states that the exponential approximation gives the best

results for the two dimensional LTS$_N$ nodal solution for deep penetration problems, we assume the ensuing approximation for the leakage angular fluxes,

$$I_{jn}(x,0) = F_{jn}e^{-sign(\mu_n)\Lambda x} \tag{24}$$

$$I_{jn}(0,y) = G_{jn}e^{-sign(\eta_n)\Lambda y} \tag{25}$$

$$I_{jn}(x,b) = O_{jn}e^{-sign(\mu_n)\Lambda x} \tag{26}$$

$$I_{jn}(a,y) = P_{jn}e^{-sign(\eta_n)\Lambda y} \tag{27}$$

where sign(μ) denotes the signal function:

$$sign(\mu) = \begin{cases} 1 & \text{if } \mu > 0 \\ -1 & \text{if } \mu > 0 \end{cases} \tag{28}$$

and Λ represents the decay constant parameter, which has to be choice a priori. In this work, we assume Λ, likewise [8], as being the absorption cross section. The functions $sign(\mu_n)$ and $sign(\eta_n)$ which appear in the equations (24) - (27) guarantee that the approximated angular fluxes will decay for any discrete direction. Replacing (24) - (27) in equations (23) and (24) the x-averaged and y-averaged angular fluxes solutions are complete after the Laplace Transform inversion. Applying the boundary conditions, we determine the integration constants and consequently the two dimensional LTS$_N$ nodal solution is well determined.

3. THE SOLUTION OF THE TWO DIMENSIONAL FOKKER-PLANCK EQUATION

In order to determine the angular flux of electrons in a rectangular domain, let us consider the following two dimensional, time independent electron transport equation [6],

$$\mu\frac{\partial\psi(x,y,\overline{\Omega},E)}{\partial x} + \eta\frac{\partial\psi(x,y,\overline{\Omega},E)}{\partial y} + \sigma_t(E)\psi(x,y,\overline{\Omega},E) = \\ = \int dE' \int_{4\pi} d\overline{\Omega}'\sigma_s(E'\rightarrow E,\overline{\Omega}'\cdot\overline{\Omega})\psi(x,y,\overline{\Omega}',E'), \tag{29}$$

in a rectangle $0 \leq x \leq a$ and $0 \leq y \leq b$, subject to vacuum boundary conditions. Here the angular flux, denoted as $\psi(x,y,E,\overline{\Omega})$, represents the flux of particles at position (x,y), with energy E travelling in direction $\overline{\Omega} = (\mu,\eta)$. The quantity σ_s in Eq. (29) is the differential scattering cross-section and is written as,

$$\sigma_s(E,\mu_0) = \frac{\sigma_t(E)\eta^*(\eta^*+1)}{\pi(1+2\eta^*-\mu_0^2)}, \tag{30}$$

where $\eta^* > 0$ is a typically small constant called the screening parameter.

Here it is important to mention that, in this work we focus on screened Rutherford scattering. Screened Rutherford scattering is one of the simplest models of elastic scattering of electrons from nuclei taking into account the screening of the nuclei by atomic electrons. It is obtained from the Schrödinger equation in the first Born approximation, using an exponential factor in the potential to model the screening effect [11]. An approximate formula for the screening parameter is written as,

$$\eta^* = \frac{h^2 Z^{\frac{2}{3}}}{4(a_H)^2(m_e v)^2}, \tag{31}$$

where Z denotes the atomic number of the nucleus, $m_e v$ is the (relativist) momentum of the electron that is being scattered, $\hbar$ is the Planck constant and a_H is the Bohr radius.

We now assume that the scattering process is sufficiently peaked in the forward direction so that the Fokker-Planck scattering description [12] is appropriate. Thus, the Fokker-Planck approximation [13] to transport problem (29) is given by,

$$\begin{aligned} \mu\frac{\partial\psi^{FP}(x,y,\overline{\Omega},E)}{\partial x} + \eta\frac{\partial\psi^{FP}(x,y,\overline{\Omega},E)}{\partial y} = \\ = \frac{\sigma_{tr}}{2}\frac{\partial}{\partial\mu}\Big[(1-\mu^2)\frac{\partial}{\partial\mu}\Big]\psi^{FP}(x,y,\overline{\Omega},E), \end{aligned} \tag{32}$$

where $\psi^{FP}(x,y,\overline{\Omega},E)$ represents the Fokker-Planck angular flux of particles at position (x,y), with energy E travelling in direction $\overline{\Omega} = (\mu,\eta)$ and the coefficient σ_{tr} is called the transport cross-section and is defined as,

$$\sigma_{tr} = 2\pi\int_{-1}^{1}\int_{0}^{1}\sigma_s(E,\mu_0)(1-\mu_0)d\mu_0 d\eta. \tag{33}$$

Multiplying the Fokker-Planck equation (32) by $P_n(\mu)$, integrating over μ, and using a recursion formula [14], we came out with the following P_N equations:

$$\begin{aligned} \frac{n+1}{2n+1}\frac{\partial}{\partial x}\psi^{FP}_{n+1}(x,y,E) + \frac{n}{2n+1}\frac{\partial}{\partial x}\psi^{FP}_{n-1}(x,y,E) + \frac{2n+1}{2}\frac{\partial}{\partial y}\psi^{FP}_{n}(x,y,E)T_n = \\ = \frac{\sigma_{tr}}{2}[-n(n+1)]\psi^{FP}_n(x,y,E), \end{aligned} \tag{34}$$

with the angular flux moments in discrete ordinates approximated by a quadrature formula as follows,

$$\psi^{FP}(x,y,\overline{\Omega},E) = \sum_{l=0}^{L}\frac{2n+1}{2}\psi^{FP}_n(x,y,E)P_n(\mu), \tag{35}$$

for $n = 0,...,N$, with $\psi^{FP}_{N+1}(x,y,E) = 0$ in the P_N approximation and T_n represented by an integral term, which can be analytic solved, written as,

$$T_n = \int_{-1}^{1}\sqrt{(1-\mu^2)}P_n(\mu)P_{n+1}(\mu)d\mu. \tag{36}$$

Once applied the Laplace transform technique in equation (34) in the spatial variable x, we came out with the following linear algebraic system in the matrix form,

$$A_n\overline{\psi_n^{FP}}'(s,y,E) + B_n(s)\overline{\psi_n^{FP}}(s,y,E) - C_n\psi_n^{FP}(0,y,E) = 0. \tag{37}$$

Here $\overline{\psi_n^{FP'}}(s,y,E)$ is the N components vector of the derivative of the angular flux Laplace transformed in the x variable with respect to y and is written as,

$$\overline{\psi_n^{FP}}'(s,y,E) = \left[\overline{\psi_0^{FP}}'(s,y,E) \quad \overline{\psi_1^{FP}}'(s,y,E) \quad ... \quad \overline{\psi_N^{FP}}'(s,y,E)\right]^T. \tag{38}$$

Here the column vector $\overline{\psi_n^{FP}}(s,y,E)$ is the N components of the angular flux Laplace transformed vector in x variable and $\psi_n^{FP}(0,y,E)$ is the N components of the angular flux vector in x variable at x = 0. They have the form:

$$\overline{\psi_n^{FP}}(s,y,E) = \left[\overline{\psi_0^{FP}}(s,y,E) \quad \overline{\psi_1^{FP}}(s,y,E) \quad ... \quad \overline{\psi_N^{FP}}(s,y,E)\right]^T, \tag{39}$$

$$\psi_n^{FP}(0,y,E) = \left[\psi_0^{FP}(0,y,E) \quad \psi_1^{FP}(0,y,E) \quad ... \quad \psi_N^{FP}(0,y,E)\right]^T. \tag{40}$$

On the other hand, the components of matrices A_n, $B_n(s)$, and C_n are given, respectively, by

$$A_n = \begin{bmatrix} 1T_0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 9T_1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 25T_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & (2N+1)^2T_N \end{bmatrix}, \tag{41}$$

$$B_n(s) = \begin{bmatrix} 0 & 2s & 0 & 0 & \cdots & 0 \\ 2s & 6\sigma_{tr} & 4s & 0 & \cdots & 0 \\ 0 & 4s & 30\sigma_{tr} & 6s & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & 2Ns \\ 0 & 0 & 0 & \cdots & 2Ns & N(N+1)(2N+1)\sigma_{tr} \end{bmatrix}, \tag{42}$$

$$C_n = \begin{bmatrix} 0 & 2 & 0 & 0 & \cdots & 0 \\ 2 & 0 & 4 & 0 & \cdots & 0 \\ 0 & 4 & 0 & 6 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 2N-2 & 0 & 2N \\ 0 & 0 & 0 & \cdots & 2N & 0 \end{bmatrix}, \tag{43}$$

where σ_{tr} and T_n are defined by Eq. (33) and Eq. (36) respectively.

The solution of equation (37) is given by,

$$\overline{\psi_n^{FP}}(s,y,E) = c1(s)\cdot e^{-\left[B_n(s)\cdot A_n^{-1}\right]y} + C_n\cdot[B_n(s)]^{-1}\cdot\psi_n^{FP}(0,y,E), \tag{44}$$

where $c_1(s)$ is an arbitrary constant. In this problem we determine the $c_1(s)$ value, by applying the boundary and interface conditions. Due to the linear character of the inverse Laplace Transform operator, taking the Laplace inversion of the above ansatz we get,

$$\psi_n^{FP}(x,y,E) = \mathcal{L}^{-1}\left\{ c1(s)\cdot e^{-\left[B_n(s)\cdot A_n^{-1}\right]y} \right\} + \\ +C_n\cdot\mathcal{L}^{-1}\left\{ [B_n(s)]^{-1} \right\}\cdot\psi_n^{FP}(0,y,E). \tag{45}$$

Once obtained the inverses matrices A_n^{-1} and $B_n^{-1}(s)$, we calculate the inversion of the first term of the equation (42) by using the Laplace convolution property. Here, it is important to mention that the inverse matrix $B_n^{-1}(s)$ wasn't obtained analytically, due to the existence of the s parameter, a non numeric parameter. Therefore, we opt to calculate the inverse Laplace transform numerically – in this work we apply the Gauss quadrature inversion method, [15, 16].

4. NUMERICAL RESULTS

In order to illustrate the aptness of the deterministic methods to solve the two dimensional transport equation for neutral and charged particles, in the sequel we report numerical simulations for the absorbed energy in rectangular domains with different dimensions and compositions. We considered a homogeneous rectangular domain composed by water, tissue or bone. We also assume a monoenergetic (E = 1.25 MeV) and monodirectional photon beam incoming on the edge of a rectangle. In this study, the energy deposited by the secondary electrons, generated by the Compton Effect, will be considered. The remaining effects will not be taken into account. The numerical results encountered for absorbed energy are compared with the ones obtained by the program Geant4.

The data were simulated using the Geant4 (version 9.1) Monte Carlo program. Just recalling, Geant4 [17] is a toolkit for simulating the passage of particles through matter. It includes a complete range of functionality including tracking, geometry, physics models and hits. The computational universe considered in this work was a monoenergetic and monodirecional source incomming in the centre line of a volume. In that way, it was possible to prevent the lost of particles on the borders, "named borders effect". For each simulation 10^6 histories were generated. In what follows, we present numerical results for the problems:

Problem 1: Let us consider a homogeneous rectangular domain, constituted by water (Z/A = 0.55508, ρ = 1 g/cm^3) and vacuum boundary condition.

In Tables 1 and 2 we present, respectively, the LTS_8 Nodal and the P_9 approximation numerical simulations for the absorbed energy in a homogeneous rectangular geometry composed by water and comparisons with the Geant4 program results. Bearing in mind that Geant4 program applies the Monte Carlo's technique, given a closer look to the results in Tables 1 and 2, we promptly realize a good coincidence. In fact, observing the results in Tables 1 and 2, we notice that the maximum discrepancy found is lower than 3% and 7%, respectively. In Tables 1a and 2a we display the numerical convergence, respectively, of the LTS_N Nodal and the P_N

Table 1. Absorbed energy [keV/photon emitted from the source] in a homogeneous rectangular domain composed by water

	Water, liquid		
Domain dimension	LTS_8	Geant4	Discrepancy
20 cm x 10 cm	0.00309	0.00315	1.9%
20 cm x 20 cm	0.00457	0.00468	2.3%
30 cm x 40 cm	0.00114	0.00116	1.7%

Table 1a. LTS_N numerical convergence

N	*20 cm x 20 cm*
2	0.00359043
4	0.00411992
6	0.00446904
8	0.00457042

Table 2. Absorbed energy [keV/photon emitted from the source] by the free electron in a homogeneous rectangular domain composed by water

	Water, liquid		
Domain dimension	P_9	Geant4	Discrepancy
20 cm x 10 cm	0.01845	0.01971	6.4%
20 cm x 20 cm	0.03379	0.03609	6.4%
30 cm x 40 cm	0.04581	0.04893	6.4%

Table 2a. P_N numerical convergence

N	*20 cm x 20 cm*
1	0.02590432
3	0.03199219
5	0.03252043
7	0.03370622
9	0.03378688

approximation results, in a rectangular domain composed by water for increasing N. In fact, observing the results in Table 1a, for $N = 6$ and $N = 8$ we notice a coincidence of one significant digits. Here, it is important to mention that the unique approximation made along the derivation of the LTS$_N$ nodal solution was in the leakage angular flux at boundary. In Table 2a, for $N = 7$ and $N = 9$, we notice a coincidence of three significant digits.

Problem 2: To check the influence of the material density in the absorbed energy calculation, let us consider a rectangular domain composed by bone cortical (Z/A = 0.51478, ρ = 1.92 g/cm^3) and vacuum boundary condition.

Table 3. Absorbed energy [keV/photon emitted from the source] in a homogeneous rectangular domain composed by bone, cortical [18]

	Bone, cortical (ICRU44)		
Domain dimension	LTS$_8$	Geant4	Discrepancy
20 cm x 10 cm	0.05588	0.05781	3.3%
20 cm x 20 cm	0.09087	0.09487	3.4%
30 cm x 40 cm	0.15771	0.16375	3.7%

Table 4. Absorbed energy [keV/photon emitted from the source] by the free electron in a rectangular domain composed by bone, cortical [18]

	Bone, cortical (ICRU44)		
Domain dimension	P$_9$	Geant4	Discrepancy
20 cm x 10 cm	0.83790	0.91244	8.2%
20 cm x 20 cm	0.79284	0.86380	8.%
30 cm x 40 cm	0.89218	0.97249	8.3%

In Tables 3 and 4 we present, respectively, the LTS$_8$ Nodal and the P$_9$ approximation numerical simulations for the absorbed energy in a rectangle composed, respectively, by bone cortical and tissue soft, and comparisons with the Geant4 program results, where the maximum discrepancy found is lower than 4% and 9%. Our numerical results demonstrate that, for higher density materials, other effects must be taken into account, because when the density is increases, the number of interaction increases as well as the possibility of other processes production involving secondary electrons. We must also mention that we have done all the LTS$_N$ nodal calculations using an AMD Athlon 1700 (1.4 GHz) microcomputer while the Geant4 results are obtained using a Pentium 4 (1.7 GHz) microcomputer. Furthermore, the maximum computational time observed to generate all the results in each table was 30 minutes for both methods: LTS$_N$ nodal solution and Monte Carlo technique.

5. CONCLUSIONS

In this work, we described the advances in a class of deterministic methods for the Boltzmann transport equation for monoenergetic problems in x,y-geometry. We must emphasize that the Fokker-Planck solution reported keeps the analytical feature, in the sense that no approximation is made along its derivation from the P_N equations, except for the round-off error. Regarding the topic of analyticity, the LTS_N nodal solution reported also keeps the analytical feature, in the sense that the unique approximation made along the derivation of the LTS_N nodal solution was in the leakage angular flux at the boundary. We must also emphasize that we attained a good agreement with the Monte Carlo technique results with a small computational effort. Bearing in mind the good agreement between the results attained by the deterministic methods described with the ones of Geant4, we are confident to stress that these methods are promising to solve the two dimensional Boltzmann transport equation for neutral and charged particles. Finally, we focus our future attention to the issue of extending the Boltzmann transport solution for two dimensional problems in a heterogeneous rectangle.

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