AN IMPROVED COMPUTATIONAL VERSION OF THE LTS_N METHOD TO SOLVE TRANSPORT PROBLEMS IN A SLAB

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Abstract. *In this work, we present an improved computational version of the LTS_N method to solve transport problems in a slab. The key feature relies on the reoerdering of the set of S_N equations. This procedure reduces by a factor of two the task of evaluating the eigenvalues of the matrix associated to SN approximations. We present numerical simulations and comparisons with the ones of the classical LTS_N approach.*

Keywords*: Discrete ordinates equations, LTS_N method, Laplace transform, Transport problems.*

1. INTRODUCTION

There is a reasonable literature regarding the issue of solving analytically the set of S_N equations. Among them we mention the LTS_N method. The motivation for this choice comes from the fact that besides the broad class of problems solved by this methodology, including multidimensional problems, this technique has also the advantage that the study of the issue of mathematical analysis concerning the subject of error bound estimate and convergence is already complete. The main idea of this method comprehends the steps: application of the Laplace transform in the spatial variable, solution of the resulting equation for the transformed angular flux and analytical Laplace transform inversion of the transformed angular flux, using the S_N matrix spectral decomposition. For a better understanding of this methodology see the works of Segatto and Vilhena (1999), Segatto *et al.* (1999b), Gonçalves *et al.* (2000) and Zabadal *et al.* (1995). In this work we step further, reporting an improved computational version of the S_N method to solve transport problems in a slab. The key feature relies on the reordering of the set of S_N equations. This procedure reduces by a factor of two the task of evaluating the eigenvalues of the matrix associated to S_N approximations. To hit this objective we organize the paper as follows: in section 2, we describe the LTS_N solution reordering the S_N equations and, in section 3, we present numerical results and comparisons with the classical LTS_N results.

2. THE COMPUTATIONAL IMPROVED LTS_N SOLUTION

We specialize the construction of the computational time improvement of the LTS_N solution for a S_N problem without azimuthal symmetry in a slab. So far, bearing in mind the Chandrasekhar decomposition approach (Chandrasekhar, 1950), the radiative transfer problem without azimuthal symmetry reduces to the solution of the following set of problems (Chalhoub and Garcia, 1997):

$$\mu\frac{\partial I_m}{\partial\tau}(\tau,\mu)+I_m(\tau,\mu)=\frac{\omega}{2}\sum_{l=m}^{L}\beta_l P_l^m(\mu)\int_{-1}^{1}d\mu' P_l^m(\mu')I_m(\tau,\mu')+Q_m(\tau,\mu), \tag{1}$$

for $m = 0, 1, \ldots, M,$ *and* $0<\tau<\tau_0$ and $\mu\in[-1,1]$, where

$$Q_m(\tau,\mu)=\frac{\omega}{2}e^{-\tau/\mu_0}\sum_{l=m}^{L}\beta_l P_l^m(\mu)P_l^m(\mu_0), \tag{2}$$

subject to the boundary conditions

$$I_m(0,\mu)=0\text{, if }\mu>0, \tag{3}$$

and

$$I_m(\tau_0,\mu)=0\text{ , if }\mu<0. \tag{4}$$

To attain the S_N approximation of Eq. (1), we expand the integral term of equation (1) by Gaussian quadrature scheme of order N ($N \geq 2$ even) and we apply the collocation method to the angular variable of $I_m(\tau,\mu)$. Here, the points of collocation, μ_n, are the N roots of the N degree Legendre polynomial, organized in decreasing order, that means, $\mu_1 > \mu_2 > \ldots > \mu_{N/2} > 0 > \mu_{N/2+1} > \ldots > \mu_N$. This procedure results in the following system of N coupled linear first order differential equations, for each $m = 0, 1, \ldots, M$:

$$\mu_n \frac{\partial I_m}{\partial \tau}(\tau,\mu_n)+I_m(\tau,\mu_n)=\frac{\omega}{2}\sum_{l=m}^{L}\beta_l P_l^m(\mu_n)\sum_{k=1}^{N} w_k P_l^m(\mu_k)\, I_m(\tau,\mu_k)+Q_m(\tau,\mu_n), \tag{5}$$

where the symbol w_n denote the weights of the Gaussian quadrature scheme. Then, recasting the set of differential equations (5) in matrix form and applying the Laplace transform technique in the spatial variable, we come out with:

$$\frac{d}{dx}\boldsymbol{I}_m(x)-\boldsymbol{A}\boldsymbol{I}_m(x)=\boldsymbol{Q}_m(x), \tag{6}$$

where the vectors $\boldsymbol{I}_m(x)$ and $\boldsymbol{Q}_m(x)$ are defined as $[I_m(x,\mu_1)\ldots I_m(x,\mu_N)]^T$ and $[Q_m(x,\mu_1)/\mu_1 \ldots Q_m(x,\mu_N)/\mu_N]^T$, respectively, and matrix $\boldsymbol{A}$ (N x N) has the entries:

$$A_{i,j}=\frac{\omega}{2\mu_i}\sum_{l=m}^{L}\beta_l P_l^m(\mu_i) w_j P_l^m(\mu_j)-\frac{1}{\mu_i}\delta_{i,j}. \tag{7}$$

The solution of this sort of problem by the LTS_N method is well known. For details see the work of Segatto *et al.* (1999b). To the computational time improvement of the LTS_N algorithm, we reorder the set of S_N equations as follows. The new set of discrete direction, $\overline{\mu}_n$, for $n = 1:N$, are defined as: $\overline{\mu}_n = \mu_n$ and $\overline{\mu}_{n+N/2} = -\mu_n$, for $n = 1:N/2$. As a consequence, Eq. (6) now reds as:

$$\frac{d}{dx}\underline{\boldsymbol{I}}_m(x)-\underline{\boldsymbol{A}}\underline{\boldsymbol{I}}_m(x)=\underline{\boldsymbol{Q}}_m(x), \tag{8}$$

where the vectors $\underline{\boldsymbol{I}}_m(x)$ and $\underline{\boldsymbol{Q}}_m(x)$ are defined like $[I_m(x,\overline{\mu}_1)\ldots I_m(x,\overline{\mu}_N)]^T$ and $[Q_m(x,\overline{\mu}_1)/\overline{\mu}_1 \ldots Q_m(x,\overline{\mu}_N)/\overline{\mu}_N]^T$, respectively. The matrix $\underline{\boldsymbol{A}}$ (N x N) has the form:

$$\underline{\boldsymbol{A}}=\begin{bmatrix} \boldsymbol{U}-\boldsymbol{B_E}-\boldsymbol{B_O} & \boldsymbol{B_O}-\boldsymbol{B_E} \\ \boldsymbol{B_E}-\boldsymbol{B_O} & \boldsymbol{B_E}+\boldsymbol{B_O}-\boldsymbol{U} \end{bmatrix}, \tag{9}$$

where the $(N/2)$ x $(N/2)$ matrices $\boldsymbol{U}$, $\boldsymbol{B_E}$ and $\boldsymbol{B_O}$ have the entries:

$$U_{i,j}=\frac{1}{\overline{\mu}_i}\delta_{i,j}, \tag{10}$$

$$(B_E)_{i,j}=\frac{\omega}{2\overline{\mu}_i}\sum_{\substack{l=m\\ l+m\ \text{even}}}^{L}\beta_l P_l^m(\overline{\mu}_i)\overline{w}_j P_l^m(\overline{\mu}_j) \tag{11}$$

and

$$(B_O)_{i,j} = \frac{\omega}{2\bar{\mu}_i} \sum_{\substack{l=m \\ l+m\ odd}}^{L} \beta_l P_l^m(\bar{\mu}_i)\bar{w}_j P_l^m(\bar{\mu}_j)\ . \tag{12}$$

To proceed the spectral decomposition of the S_N matrix, we mean $\underline{\boldsymbol{A}} = \underline{\boldsymbol{X}}\,\underline{\boldsymbol{D}}\,\underline{\boldsymbol{X}}^{-1}$, we must observe the symmetry of the eigenvalues of matrix $\underline{\boldsymbol{A}}$, appearing in equation (9). From this fact, the matrix **D** is promptly written as block matrix like:

$$\underline{\boldsymbol{D}} = \begin{bmatrix} -\boldsymbol{\Delta} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Delta} \end{bmatrix}. \tag{13}$$

In addition the matrix **X** has the form

$$\underline{\boldsymbol{X}} = \begin{bmatrix} \boldsymbol{X}_{11} & \boldsymbol{X}_{12} \\ \boldsymbol{X}_{21} & \boldsymbol{X}_{22} \end{bmatrix}. \tag{14}$$

To solve the eigenvalue problem, we consider the problem $\underline{\boldsymbol{A}}\,\underline{\boldsymbol{X}} = \underline{\boldsymbol{X}}\,\underline{\boldsymbol{D}}$. Indeed, we determine the eigenvalues by solving the following equations:

$$\begin{cases} (\boldsymbol{U} - \boldsymbol{B_E} - \boldsymbol{B_O})\boldsymbol{X}_{11} - (\boldsymbol{B_E} - \boldsymbol{B_O})\boldsymbol{X}_{21} = -\boldsymbol{X}_{11}\boldsymbol{\Delta} \\ (\boldsymbol{U} - \boldsymbol{B_E} - \boldsymbol{B_O})\boldsymbol{X}_{12} - (\boldsymbol{B_E} - \boldsymbol{B_O})\boldsymbol{X}_{22} = \boldsymbol{X}_{12}\boldsymbol{\Delta} \\ (\boldsymbol{B_E} - \boldsymbol{B_O})\boldsymbol{X}_{11} - (\boldsymbol{U} - \boldsymbol{B_E} - \boldsymbol{B_O})\boldsymbol{X}_{21} = -\boldsymbol{X}_{21}\boldsymbol{\Delta} \\ (\boldsymbol{B_E} - \boldsymbol{B_O})\boldsymbol{X}_{12} - (\boldsymbol{U} - \boldsymbol{B_E} - \boldsymbol{B_O})\boldsymbol{X}_{22} = \boldsymbol{X}_{22}\boldsymbol{\Delta} \end{cases}. \tag{15}$$

After making some algebraic operations, we straightly come out with the following set of equations that will allow us to determine eigenvalues and the eigenvectors:

$$(\boldsymbol{U} - 2\boldsymbol{B_O})(\boldsymbol{U} - 2\boldsymbol{B}_E)\boldsymbol{\Gamma} = \boldsymbol{\Gamma}\boldsymbol{\Delta}^2\ . \tag{16}$$

Whose solution is the eigenvalue matrix $\boldsymbol{\Delta}^2$ and the eigenvector matrix $\boldsymbol{\Gamma}$, given by

$$\boldsymbol{\Gamma} = \boldsymbol{X}_{11} + \boldsymbol{X}_{21} = \boldsymbol{X}_{21} + \boldsymbol{X}_{22} \tag{17}$$

and

$$(\boldsymbol{U} - 2\boldsymbol{B}_E)\boldsymbol{\Gamma}\boldsymbol{\Delta}^{-1} = \boldsymbol{X}_{11} - \boldsymbol{X}_{21} = \boldsymbol{X}_{21} - \boldsymbol{X}_{22}\ . \tag{18}$$

Thus, solving the Eq. (16), we obtain the diagonal matrix $\underline{\boldsymbol{D}}$ from Eq. (13) and the eigenvector matrix is written as:

$$\underline{\boldsymbol{X}} = \begin{bmatrix} \dfrac{\boldsymbol{\Gamma} - (\boldsymbol{U} - 2\boldsymbol{B}_E)\boldsymbol{\Gamma}\boldsymbol{\Delta}^{-1}}{2} & \dfrac{\boldsymbol{\Gamma} + (\boldsymbol{U} - 2\boldsymbol{B}_E)\boldsymbol{\Gamma}\boldsymbol{\Delta}^{-1}}{2} \\ \dfrac{\boldsymbol{\Gamma} + (\boldsymbol{U} - 2\boldsymbol{B}_E)\boldsymbol{\Gamma}\boldsymbol{\Delta}^{-1}}{2} & \dfrac{\boldsymbol{\Gamma} - (\boldsymbol{U} - 2\boldsymbol{B}_E)\boldsymbol{\Gamma}\boldsymbol{\Delta}^{-1}}{2} \end{bmatrix}. \tag{19}$$

Finally, to invert the matrix $\underline{\boldsymbol{X}}$, we consider:

$$\underline{\boldsymbol{X}}^{-1} = \begin{bmatrix} \boldsymbol{Y}_{11} & \boldsymbol{Y}_{12} \\ \boldsymbol{Y}_{21} & \boldsymbol{Y}_{22} \end{bmatrix} \tag{20}$$

and solve the equation $\underline{\boldsymbol{X}}.\underline{\boldsymbol{X}}^{-1} = \boldsymbol{I}$, where $\boldsymbol{I}$ denotes the identity matrix of order $N/2$, obtaining the solution:

$$X^{-1} = \begin{bmatrix} \dfrac{\Gamma^{-1} - \Delta[(U - 2B_E)\Gamma]^{-1}}{2} & \dfrac{\Gamma^{-1} + \Delta[(U - 2B_E)\Gamma]^{-1}}{2} \\ \dfrac{\Gamma^{-1} + \Delta[(U - 2B_E)\Gamma]^{-1}}{2} & \dfrac{\Gamma^{-1} - \Delta[(U - 2B_E)\Gamma]^{-1}}{2} \end{bmatrix}. \tag{21}$$

Thus, we can attain the diagonalization of the *NxN* matrix $\underline{\boldsymbol{A}}$, where the matrices $\underline{\boldsymbol{D}}$, $\underline{\boldsymbol{X}}$ and its inverse by Eqs. (14), (19) e (21), respectively, reducing this problem to the *(N/2) x (N/2)* eigenvector problem given by Eq. (16). Then, having $\underline{A} = \underline{X}\,\underline{D}\,\underline{X}^{-1}$, we solve Eq. (8) by the LTS_N method (Segatto *et al.*, 1999b), resulting the following solution:

$$\begin{aligned} I_m(\tau,\mu_n) = \sum_{i=1}^{N/2} \Big\{ & \alpha(n,i)e^{d(i)\tau}\xi_m^i + \alpha(n,i+N/2)e^{d(i+N/2)(\tau-\tau_0)}\xi_m^{i+N/2} \\ & + \sum_{j=1}^{N}\Bigg[\frac{\alpha(n,i)\alpha^{-1}(i,j)}{\mu_j}\int_0^{\tau} e^{d(i)(\tau-x)}Q_m(x,\mu_j)dx \\ & + \frac{\alpha(n,i+N/2)\alpha^{-1}(i+N/2,j)}{\mu_j}\int_{\tau_0}^{\tau} e^{d(i+N/2)(\tau-x)}Q_m(x,\mu_j)dx\Bigg]\Bigg\} \end{aligned}, \tag{22}$$

where $\alpha(i,j)$ and $\alpha^{-1}(i,j)$ are, respectively the entries of the eigenvector matrix $\underline{\boldsymbol{X}}$ and its inverse $\underline{\boldsymbol{X}}^{-1}$. The coefficients *d(i)* are the eigenvalues of the matrix $\underline{\boldsymbol{A}}$. The unknown constants (ξ_m^i) are determined by the application of the boundary conditions (3-4) at the discrete directions.

3. NUMERICAL RESULTS AND FINAL CONSIDERATIONS

In order to verify the aptness of this improved, we solve a test problem proposed by the Radiation Commission of the International Association of Meteorology and Atmospheric Physics (Lenoble, 1977), based in a haze L scattering model: anisotropic scattering of degree $L = 82$, $\tau_0 = 1$, $\omega = 0.9$ and $\mu_0 = 0.5$, and the β_l parameters depicted in table 10 of Garcia and Siewert (1985). In Tabs. 1-2 we display respectively the classical and computational improved LTS_N results for different values of the angular variable μ for the uncollided angular intensity, expressed like:

$$I_*(\tau,\mu,\varphi) = \frac{1}{2}\sum_{k=0}^{L}(2-\delta_{k,0})I_k(\tau,\mu)\cos[k(\varphi-\varphi_0)], \tag{23}$$

Table 1. The Intensity $I_*(\tau,\mu,\varphi)$ for the Haze L Phase Function with $\tau_0 = 1,\ \omega = 0.9,\ \mu_0 = 0.5$ and $\phi - \phi_0 = 0$ using the LTS_{500} method.

	τ = 0	τ = τ₀/20	τ = τ₀/10	τ = τ₀/5	τ = τ₀/2	τ = 3τ₀/4	τ = τ₀
-0.9	4.11125E-02	3.86277E-02	3.60559E-02	3.08703E-02	1.64542E-02	6.81045E-03	-
-0.8	6.49980E-02	6.12970E-02	5.73956E-02	4.93999E-02	2.66076E-02	1.10212E-02	-
-0.7	9.99442E-02	9.47419E-02	8.91208E-02	7.73507E-02	4.26130E-02	1.79326E-02	-
-0.6	1.50993E-01	1.44083E-01	1.36343E-01	1.19657E-01	6.81167E-02	2.95063E-02	-
-0.5	2.24767E-01	2.16263E-01	2.06169E-01	1.83479E-01	1.09067E-01	4.93121E-02	-
-0.4	3.29333E-01	3.20181E-01	3.08044E-01	2.78888E-01	1.75209E-01	8.41048E-02	-
-0.3	4.72532E-01	4.65519E-01	4.52953E-01	4.18718E-01	2.82081E-01	1.47238E-01	-
-0.2	6.56828E-01	6.58389E-01	6.49494E-01	6.15206E-01	4.51465E-01	2.66181E-01	-
-0.1	8.70307E-01	8.94523E-01	8.97444E-01	8.72171E-01	6.97514E-01	4.91553E-01	-
0.1	-	6.07537E-01	9.98585E-01	1.38472E+00	1.41181E+00	1.15806E+00	8.76461E-01
0.2	-	5.08877E-01	9.07218E-01	1.43790E+00	1.82630E+00	1.61272E+00	1.29143E+00
0.3	-	5.49992E-01	9.99895E-01	1.64825E+00	2.30786E+00	2.15587E+00	1.80549E+00
0.4	-	6.38614E-01	1.16925E+00	1.95778E+00	2.87301E+00	2.77822E+00	2.40104E+00
0.5	-	6.34270E-01	1.16869E+00	1.98320E+00	3.03333E+00	3.03426E+00	2.71054E+00
0.6	-	4.18259E-01	7.78087E-01	1.34620E+00	2.18395E+00	2.29506E+00	2.15369E+00
0.7	-	2.04883E-01	3.85810E-01	6.83932E-01	1.19334E+00	1.33200E+00	1.32682E+00
0.8	-	8.64751E-02	1.65150E-01	3.01013E-01	5.69583E-01	6.78608E-01	7.19934E-01
0.9	-	3.13663E-02	6.09009E-02	1.14612E-01	2.37335E-01	3.03207E-01	3.43478E-01

for N = 500. We evaluate the angular intensity at directions appearing in Tabs. 1 and 2 performing a cubic spline interpolation. We made all the calculations with a Pentium III 400 MHz microcomputer and we observed a gain at the computational time from the improved LTS_N approach, in relation to the classical LTS_N method, from 1345.2 seconds to 1825.9 seconds.

Table 2. The Intensity $I_*(\tau, \mu, \varphi)$ for the Haze L Phase Function with
$\tau_0 = 1, \omega = 0.9, \mu_0 = 0.5$ and $\phi - \phi_0 = 0$ using the improved version of the LTS_{500} method.

	τ = 0	**τ = τ₀/20**	**τ = τ₀/10**	**τ = τ₀/5**	**τ = τ₀/2**	**τ = 3τ₀/4**	**τ = τ₀**
-0.9	4.11125E-02	3.86277E-02	3.60559E-02	3.08703E-02	1.64542E-02	6.81045E-03	-
-0.8	6.49980E-02	6.12970E-02	5.73956E-02	4.93999E-02	2.66076E-02	1.10212E-02	-
-0.7	9.99442E-02	9.47419E-02	8.91208E-02	7.73507E-02	4.26130E-02	1.79326E-02	-
-0.6	1.50993E-01	1.44083E-01	1.36343E-01	1.19657E-01	6.81167E-02	2.95063E-02	-
-0.5	2.24767E-01	2.16263E-01	2.06169E-01	1.83479E-01	1.09067E-01	4.93121E-02	-
-0.4	3.29333E-01	3.20181E-01	3.08044E-01	2.78888E-01	1.75209E-01	8.41048E-02	-
-0.3	4.72532E-01	4.65519E-01	4.52953E-01	4.18718E-01	2.82081E-01	1.47238E-01	-
-0.2	6.56828E-01	6.58389E-01	6.49494E-01	6.15206E-01	4.51465E-01	2.66181E-01	-
-0.1	8.70307E-01	8.94523E-01	8.97444E-01	8.72171E-01	6.97514E-01	4.91553E-01	-
0.1	-	6.07537E-01	9.98585E-01	1.38472E+00	1.41181E+00	1.15806E+00	8.76461E-01
0.2	-	5.08877E-01	9.07218E-01	1.43790E+00	1.82630E+00	1.61272E+00	1.29143E+00
0.3	-	5.49992E-01	9.99895E-01	1.64825E+00	2.30786E+00	2.15587E+00	1.80549E+00
0.4	-	6.38614E-01	1.16925E+00	1.95778E+00	2.87301E+00	2.77822E+00	2.40104E+00
0.5	-	6.34270E-01	1.16869E+00	1.98320E+00	3.03333E+00	3.03426E+00	2.71054E+00
0.6	-	4.18259E-01	7.78087E-01	1.34620E+00	2.18395E+00	2.29506E+00	2.15369E+00
0.7	-	2.04883E-01	3.85810E-01	6.83932E-01	1.19334E+00	1.33200E+00	1.32682E+00
0.8	-	8.64751E-02	1.65150E-01	3.01013E-01	5.69583E-01	6.78608E-01	7.19934E-01
0.9	-	3.13663E-02	6.09009E-02	1.14612E-01	2.37335E-01	3.03207E-01	3.43478E-01

From the above results we readily notice a reasonable computational improvement of the reported LTS_N version results. In fact, we notice roughly speaking, besides the very good agreement, a reduction of about 25% of the computational time, in comparison with the classical LTS_N results. From this fact, we have confidence to affirm that the mathematical analysis of the LTS_N is complete in sense that we fulfill the task of the LTS_N solution construction with computational time improvement, study of error bounded estimate and convergence as well applications to a broad class of problems including multidimensional ones. We finalize, pointing out that the LTS_N method is an efficient, robust and consequently promising method to solve and generate benchmark results to transport problem in a slab.

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