Some Equations of Discrete Space Method (DSM) for Polarized Line Transfer

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Abstract. In this note, we present few equations of the Discrete Space Method (DSM) for polarized line transfer. These equations are presented as extensions to the main paper entitled *Numerical Solutions of Polarized Line Transfer Equations*, presented in these Proceedings.

1. Introduction

The DSM is a finite difference, discrete ordinate method. Full set of equations of the DSM for polarized line transfer are derived in Nagendra (1986, 1988). The method presented there can be employed for solving transfer problems with CRD or PRD line scattering in static, axi-symmetric, 1D planar or spherical media. For simplicity, we present in this note the equations relevant to a static planar slab case. Extensive discussions on DSM is also given in Peraiah (2001).

The Finite Difference Discretization of the Medium:
We divide the medium into N-layers of arbitrary optical thickness. See Fig. (1) for spatial discretization of a planar medium. Our purpose is to compute the reflection (r) and transmission (t) operators for each layer.

The Forward Elimination Process in DSM to compute Global Operators:
The non-local r and t operators are computed during forward elimination process by applying the boundary conditions at $n = 1$ (top of the atmosphere)

$$r(1,1) = 0; \qquad V_{\frac{1}{2}}^{+} = I_{\text{incident}}^{+}(\tau = 0, \ +\mu), \tag{1}$$

and computing recursively, for $n = 1, 2, 3, ..., N$, following non-local operators

$$r(1, n+1) = r(n, n+1) + t(n+1, n) \, r(1, n) \left[I - r(n+1, n)r(1, n)\right]^{-1} t(n, n+1), \tag{2}$$

$$V_{n+\frac{1}{2}}^{+} = \hat{t}(n+1, n) \, V_{n-\frac{1}{2}}^{-} + \Sigma^{+}(n+1, n) + R_{n+\frac{1}{2}} \, \Sigma^{-}(n, n+1) , \tag{3}$$

$$V_{n+\frac{1}{2}}^{-} = \hat{r}(n+1, n) \, V_{n-\frac{1}{2}}^{+} + T_{n+\frac{1}{2}} \, \Sigma^{-}(n, n+1) . \tag{4}$$

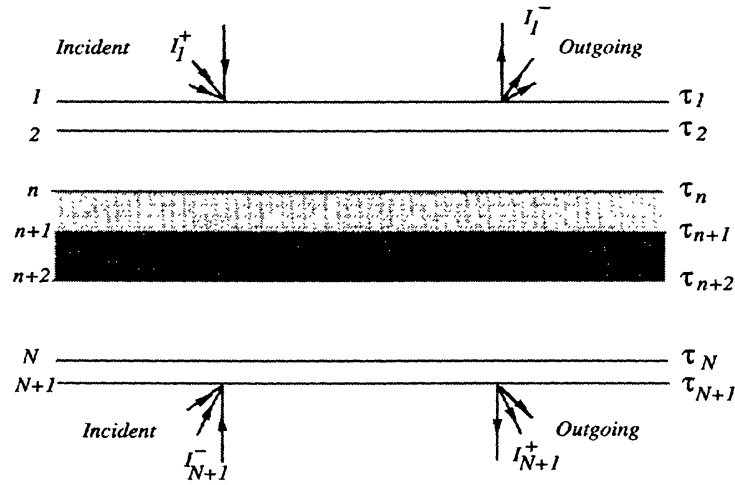In these equations, the auxiliary quantities are:

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Figure 1.   The division of the medium into layers of arbitrary optical thickness. $\tau_1 \approx 10^{-2}$ represents the top of the atmosphere. When thickness of the layer $(n, n+1)$ exceeds the 'critical optical depth', a doubling method is used to generate the 'thick layer operators', actually starting from operators for the fundamental sub-layer within the concerned layer, whose thickness is taken to be smaller than or equal to the critical optical depth.

$$\hat{t}(n+1, n) = t(n+1, n) [I - r(1, n) r(n+1, n)]^{-1} , \qquad (5)$$

$$\hat{r}(n+1, n) = r(n+1, n) [I - r(1, n) r(n+1, n)]^{-1} , \qquad (6)$$

$$R_{n+\frac{1}{2}} = \hat{t}(n+1, n) r(1, n) [I - r(1, n) r(n+1, n)]^{-1}, \qquad (7)$$

$$T_{n+\frac{1}{2}} = [I - r(n+1, n) r(1, n)]^{-1} , \qquad (8)$$

$$\hat{t}(n, n+1) = T_{n+\frac{1}{2}} t(n, n+1) . \qquad (9)$$

In the terms of the type $t(n+1, n) r(1, n) [I - r(n+1, n) r(1, n)]^{-1} t(n, n+1)$ (the second term on the r.h.s of Eq. (2)), the presence of multiple scattering is noticed by expanding the square bracket in a Taylor series.

Back Substitution Process in DSM to compute the Radiation Field:
Back substitution is necessary to compute the intensities at all the shell boundaries. This is done by applying the boundary conditions at $n = N$ (bottom of the atmosphere)

$$I_{N+1}^- = I_{\text{incident}}^- (\tau = T, -\mu), \qquad (10)$$

and computing recursively, for $n = N, \ N-1, \ N-2, ..., 2, 1$ the outgoing (-) and incoming (+) radiation from every layer $(n, n+1)$ of the atmosphere

$$I_{n+1}^+ = r(1, n+1) I_{n+1}^- + V_{n+\frac{1}{2}}^+ , \tag{11}$$

$$I_n^- = \hat{t}(n, n+1) I_{n+1}^- + V_{n+\frac{1}{2}}^- . \tag{12}$$

A Note on the Critical Optical Depth:
The square matrices $t(n+1, n)$, $t(n, n+1)$, $r(n+1, n)$, $r(n, n+1)$ are reflection and transmission operators for each layer $(n, n+1)$. However, if the atmospheric layer thickness exceeds critical optical depth $\Delta\tau_{\text{crit}}$ of the basic computational cell, then we employ van de Hulst's high speed doubling process to generate thick shell r and t operators. The critical optical depth for the basic cell $\Delta\tau_{\text{crit}}$ strongly depends on the redistribution function, the phase matrix, the angular, frequency, and geometric variables etc. It is pre-computed and used in calculating r and t operators of the basic computational cell. As long as the necessary condition

$$\Delta\tau_{\text{ basic cell}}(n, n+1) \leq \Delta\tau_{\text{crit}}(n, n+1), \tag{13}$$

is strictly satisfied, numerical stability of solution by DSM is guaranteed.

Computation of the Fundamental Cell Operators:
The following algorithm can be used to compute cell operators, in axi-symmetric planar slab cases:

$$G^\pm = [I - g^\pm g^\mp]^{-1}; \qquad g^\pm = \frac{\tau}{2}\Delta^\pm Y_\mp; \tag{14}$$

$$Z_\pm = \Phi^\pm - \frac{\delta}{2}R^{\pm,\pm}W^{\pm,\pm}; \qquad Y_\pm = \frac{\delta}{2}R^{\mp,\pm}W^{\mp,\pm} \tag{15}$$

$$D = M - \frac{\tau}{2}Z_-; \qquad A = M - \frac{\tau}{2}Z_+; \qquad \Delta^\pm = [M + \frac{\tau}{2}Z_\pm]^{-1} \tag{16}$$

The transmission, reflection and source operators are

$$t(n+1, n) = G^+[\Delta^+ A + g^+ g^-]; \qquad t(n, n+1) = G^-[\Delta^- D + g^- g^+] \tag{17}$$

$$r(n+1, n) = G^- g^-[I + \Delta^+ A]; \qquad r(n, n+1) = G^+ g^+[I + \Delta^- D] \tag{18}$$

$$\Sigma^+(n+1, n) = G^+[\Delta^+ S^+ + g^+ \Delta^- S^-]\tau; \quad \Sigma^-(n, n+1) = G^-[\Delta^- S^- + g^- \Delta^+ S^+]\tau \tag{19}$$

The auxiliary quantities in the above equations are:

$$M = [\mu_j \delta_{k,k'}]; \quad k = j + (i-1) * J + (p-1) * IJ; \quad 1 \leq k \leq PIJ, \tag{20}$$

with P, I, and J being running indices. P is the number of polarization states considered (2, 3, 4, or 6). J and I are the number of angle (μ) and frequency (x) points of the respective quadratures. Further,

$$\Phi^{\pm} = [\beta + \phi_k^{\pm}]\delta_{k,k'} \quad \text{with} \quad \phi_k^{\pm} = \phi(x_i, \pm\mu_j); \quad \text{and} \quad S^{\pm} = [\beta + \varepsilon\phi_k^{\pm}]B_{n+\frac{1}{2}}\delta_{k,k'}\hat{1},$$

$$(21)$$

where, ϕ represents the profile function; and S the thermal source matrix. The quantity $\hat{1}$ is a unity matrix with first IJ elements equal to 1, and the rest being zero. B represents local Planck function. The discrete representation of redistribution matrices and the renormalised quadrature weights matrix is

$$R^{\pm,\pm} = [R_{k,k'}^{\pm,\pm}] = R(x_i, \pm\mu_j, p;\ x_{i'}, \pm\mu_{j'}, p'); \qquad W^{\pm,\pm} = [\bar{a}_i^{\pm,\pm}c_j\delta_{k,k'}], \quad (22)$$

where $\bar{a}$ means re-normalized frequency weights. For further details regarding these numerical points see Peraiah (2001). The main steps are listed below.

The Main steps of the DSM Method:

• Step 1: Integrate transfer equation in the 1st order differential form, over a basic 'computational cell'. For example, the computational cell in the case of line transfer equation in spherical Co-Moving Frame (CMF) is $[r_n,\ r_{n+1}] \times [\mu_{j-\frac{1}{2}},\ \mu_{j+\frac{1}{2}}] \times [\nu_{i-\frac{1}{2}},\ \nu_{i+\frac{1}{2}}]$ representing $[\partial I/\partial r] \times [\partial I/\partial \mu] \times [\partial I/\partial \nu]$.

• Step 2: Define 'cell averages' of the physical and geometric variables – eg., the diamond scheme: $\tau_{n+1/2} = \frac{1}{2}(\tau_n + \tau_{n+1});\quad B_{n+1/2} = \frac{1}{2}(B_n + B_{n+1})$, etc..

• Step 3: Step 1 + Step 2 lead to a fully discretized form of RTE, which can be organized in matrix difference equation form.

• Step 4: Compute the 'fundamental cell (layer) operators', and if the atmospheric layer is optically thick (say in the denser part of the medium), then compute the 'thick layer operators' for each layer, bounded by $(n, n+1)$.

• Step 5: Arrange these matrix equations in the form of a global 'interaction principle' (namely in a canonical form). This is called 'forward elimination process' to construct global (or non-local) operators.

• Step 6: Apply the initial and boundary conditions, and perform 'back substitution' to compute the internal and emergent diffuse radiation field.

Computational Aspects of the Discrete Space Method:
(1) A finite difference discrete ordinate representation is employed to replace the derivatives and integrals. The accuracy of normalization conditions, and the final solution depend on the schemes used, and the degree of resolution employed. Gaussian quadrature for angles, logarithmic spatial grid, logarithmically spaced weighted Simpson, or spline frequency quadrature weights, are good in most cases. (2) The DSM is of linear accuracy in τ- variable. But, it is highly accurate in practical NLTE work, because we use very small values of $\Delta\tau_{\text{crit}}$ as the basic cell thickness, and employ highly accurate and efficient doubling method of van de Hulst to generate the r, t and Σ operators for the

whole thick layer $(n, n+1)$. **(3)** The main effort goes in computing the cell matrices r and t for each layer of the the atmosphere. Depending on the physical nature of the problem, and the geometry (planar, spherical, and multi-D media), it requires less or more CPU time. **(4)** The generation of global operators $r(1, n+1)$, $\hat{t}(n, n+1)$ and $V^{\pm}_{n+\frac{1}{2}}$ representing the entire atmosphere, also involves large computing efforts. **(5)** Considerably large main memory is required to store the $r(1, n+1)$, $\hat{t}(n, n+1)$ and $V^{\pm}_{n+\frac{1}{2}}$ operators for all the shells, or a large CPU time is expended in doing the I/O operations if one employs a secondary storage on hard disk.

Advantages and Disadvantages of the Discrete Space Method:
The advantages are:
(1) Clarity in the generalization of the DSM to more and more complex physical problems (in practical terms, the ease of numerical extension), **(2)** High accuracy and stability of the numerical solutions, **(3)** Possibility of self-consistency checks like 'flux conservation', 'constancy of net flux in conservative scattering media', etc., to ensure correct coding and accuracy of the discrete representation. **(4)** Easy parallelization and vectorizability of the code. **(5)** DSM is suitable for exploratory work involving new physical effects, and generate benchmarks to serve as checks for other numerical methods like PALI.

The main disadvantage is:
Generalization to non-axisymmetric problems (like Hanle effect), by direct discretization over the azimuth angle φ; or, generalization to multi-D by direct discretization over spatial variables, or application to realistic atmospheric modeling work, leads to increased dimensionality of the matrices in the algorithm leading to large memory and CPU time requirement. Clearly, approximate methods are preferable for non-axisymmetric, or multi-D polarized line transfer applications, or in the atmospheric modeling work.

References

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