

**SWEEP-BY-SWEEP IMPLICIT LAMBDA
ITERATION FOR NON-LTE RADIATIVE
TRANSFER IN 2D CARTESIAN COORDINATES**

I. MILIĆ¹ and O. ATANACKOVIĆ²

¹*Astronomical Observatory, Volgina 7, 11060 Belgrade, Serbia*
E-mail: milic@aob.rs

²*Faculty of Mathematics, University of Belgrade, Studentski Trg 16, 11000 Belgrade, Serbia*
E-mail: olga@matf.bg.ac.rs

Abstract. We have recently developed a novel method for solving non-LTE radiative transfer problem in 2D media. The method can be considered as a generalization of the Forth-and-back implicit lambda iteration (FBILI), originally developed for 1D atmospheric models. In this so-called Sweep-by-sweep implicit lambda iteration short characteristics approach is used for the formal solution of the radiative transfer equation, whereas an extremely high convergence rate is achieved by means of multiple source function updates within one iteration and thanks to the use of quasi-invariant iteration factors. In this paper we briefly present its implementation in the case of two-level atom line transfer with complete frequency redistribution in a 2D Cartesian grid and we compare its convergence properties with those of the iterative methods currently in use (Jacobi and Gauss-Seidel iteration). We show that Sweep-by-sweep ILI converges 6-7 times faster than the Jacobi method and scales better with grid resolution.

1. INTRODUCTION

The aim of radiative transfer modeling is to properly treat the interplay between the radiation field and the matter, with the ultimate purpose of self-consistent modeling of various astrophysical objects. It is a challenging task both conceptually (different physical processes on various geometrical scales are involved) and numerically. This is so even in the so-called “reduced” problem of computing the emergent spectrum from a given model. Assuming the non-local thermodynamic equilibrium (NLTE) we are faced with the self-consistent solution of both the radiative transfer (RT) and the statistical equilibrium (SE) equations for the unknown radiation field and the atomic level populations. In general, the NLTE problem is non-local and non-linear and requires immense computational power for its solution.

A “classical” radiative transfer computations assume one-dimensional models where all quantities depend on only one spatial coordinate. The problem and the solutions are given in the excellent monograph by Mihalas (1978). However, there are many objects like solar prominences, accretion and circumstellar disks and rings, various kinds

of jets, etc., for which 1D approximation is not adequate. Stellar atmospheres themselves are also highly inhomogeneous objects where lateral (i.e. horizontal) radiative transfer effects must not be neglected if we are to compute the emergent spectrum properly. However, 2D or 3D NLTE modeling is numerically much more intensive, and apart from parallelization strategies (see, e.g. Štepan & Trujillo Bueno, 2013), faster methods for the solution of the multidimensional NLTE problem are needed.

Here, we present our recent work on the generalization of Forth-and-back Implicit Lambda Iteration (FBILI, Atanacković-Vukmanović et al., 1997) to 2D Cartesian geometry. The basic equations of the problem are given in Section 2. In Section 3 we outline a variant of the short characteristics approach to the formal solution of the RT equation and its use in four iterative schemes: Jacobi method, Gauss-Seidel method, the Symmetric Gauss-Seidel iteration (SGS, not yet generalized to multidimensional geometries), and the Sweep-by-sweep Implicit Lambda Iteration (SsILI). In Section 4 we discuss the convergence and scaling properties of the iterative procedures, demonstrating the superiority of SsILI method. In Conclusions we give some possible directions for the future work.

2. NLTE PROBLEM

Here, we shall restrict ourselves to two-level atom line transfer with complete frequency redistribution and no background continuum in a static medium. If we assume that the medium is infinite and homogeneous in the z-direction, the RT equation has the following form:

$$\frac{dI(x, y, \hat{\Omega}, \nu)}{d\tau} = \phi(x, y, \nu) [I(x, y, \hat{\Omega}, \nu) - S(x, y)]. \quad (1)$$

Here, $I(x, y, \hat{\Omega}, \nu)$ is the specific intensity at the chosen spatial point (x, y) , in direction $(\hat{\Omega})$ and at frequency (ν) , τ is the line-integrated optical path, $\phi(x, y, \nu)$ is the line absorption profile, and $S(x, y)$ is the line source function given as:

$$S(x, y) = \epsilon(x, y)B_P(x, y) + (1 - \epsilon(x, y))J(x, y). \quad (2)$$

In the above expression, B_P is the Planck function, $\epsilon = C_{ul}/(C_{ul} + A_{ul})$ is the photon destruction probability by collisional de-excitation, with C_{ul} and A_{ul} - collisional and radiative rates from the upper to the lower level of the transition, respectively, and

$$J(x, y) = \int_{-\infty}^{\infty} \phi(x, y, \nu) d\nu \oint I(x, y, \hat{\Omega}, \nu) \frac{d\hat{\Omega}}{4\pi}. \quad (3)$$

is the scattering integral. Equations 1 and 2 are linearly coupled. In the case of the multilevel atom line transfer the coupling is non-linear and has to be treated iteratively. With the final aim to solve this general problem, first we develop the iterative procedures and test their properties using a simple two-level atom case for which the exact solution is known. First we shall present the *formal solution*, i.e. a way of computing the specific intensity with the given source function as it is the backbone of each iterative technique, and then we shall briefly describe its use in the four above mentioned iterative procedures.

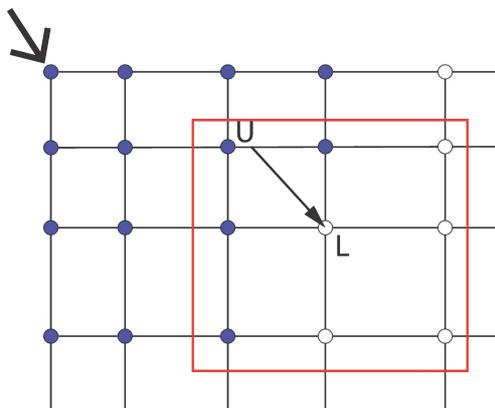


Figure 1: Example of one sweep of the spatial mesh. Full points are the ones where the formal solution has been performed and specific intensity is known while the empty ones are the ones where the formal solution is yet to be performed. Note that this implies the specific order in which the formal solution is done. The square emphasizes the source functions which contribute to the specific intensity at the local point.

3. METHOD OF SOLUTION

Proceeding from the integral form of the RT equation, we can see that the specific intensity at a given point $L = (i, j)$, in the given direction and at the given frequency can be expressed as (see Milić & Atanacković, 2014):

$$I_L = I_U e^{-\Delta} + p(\Delta) S_L + \sum_{i'-1}^{i+1} \sum_{j'-1}^{j+1} r_{i'j'}(\Delta) S_{i'j'}. \quad (4)$$

Here I_U is the specific intensity in the same direction and at the same frequency, but at the “upwind” point, i.e. the point of the first intersection between the ray and the grid, in the direction opposite to that of photon propagation. Since the point U is not on the spatial grid, I_U has to be found by spatial interpolation. Δ is the monochromatic optical path between U and L , S_L is the “local” source function and the sum accounts for the contributions of the eight nearby source functions to the local specific intensity ($i' = i - 1, i, i + 1, j' = j - 1, j, j + 1, r_{ij} = 0$). For the formal solution in a given direction, one has to start from the corresponding given boundary condition and “sweep” the grid in the appropriate order (Fig.1). For example, if the angle ϕ in the x, y plane has values $0 < \phi < \pi/2$, one has to start from boundaries $x = 0$ and $y = 0$. We will refer to the computations of the specific intensities for a given quadrant of ϕ as one sweep. In 1D case there are two sweeps (“in-going” and “out-going”), in 2D case there are four, and in 3D there are eight sweeps of the grid.

If we now integrate Eq. (4) over angles and line profile we get:

$$J_L = a + b S_L + \sum_{i'-1}^{i+1} \sum_{j'-1}^{j+1} c_{i'j'} S_{i'j'}. \quad (5)$$

Even if we know neither radiation field nor the source function, the fact that we can write an implicit linear relation (like Eq. 5) between these unknowns enables the construction of the efficient iterative procedures to solve the problem equations (1) and (2).

We see that substituting Eq. (5) into Eq. (2) we get the expression for updating the source function

$$S = \frac{\epsilon B_P + (1 - \epsilon)(a + \sum_{i=1}^{i+1} \sum_{j=1}^{j+1} c_{i'j'}(\Delta) S_{i'j'})}{1 - (1 - \epsilon)b} \quad (6)$$

once all the coefficients a , b , $c_{i'j'}$ are known. The use of the above implicit linear relation instead of iterative computation of the unknown quantities themselves (as in the classical Λ iteration) greatly increases the convergence rate.

3. 1. ITERATIVE SCHEMES

The most straightforward accelerating iterative procedure performs formal solution in all directions, at all frequencies and over the whole grid in order to compute the coefficients a , b and c and then use them in Eq. (6) to update the values of the source function. This corresponds to the well-known Jacobi method (see e.g. Saad, 2003). Note that the source function is then updated *after* all four sweeps of the grid. Substantial acceleration can be obtained if the source function is updated *in the course of* the fourth sweep, that is, as soon as a , b and c coefficients are known. This procedure corresponds to the Gauss-Seidel method, which has been used in 1D NLTE radiative transfer computations by Trujillo Bueno & Fabiani Bendicho (1995) and extended to 2D by Paletou & Leger (2007). The GS approach can be further accelerated if, after the first iteration, the update of the source function is performed during *each* sweep (that is, four times per iteration). This procedure corresponds to the symmetric Gauss-Seidel (SGS) method, which (to our knowledge) was first generalized to multidimensional radiative transfer computations in the paper by Milić & Atanacković (2014).

Finally, even further acceleration is possible by the use of the iteration factors together with the implicit treatment of the source function and its derivatives (through the sum of eight neighboring source functions in Eq. 5) based on the ideas introduced for 1D NLTE radiative transfer by Atanacković-Vukmanović et al. (1997) in the framework of FBILI. Thus, proceeding from the form of Eq. (5) we introduce the ratio of the non-local intensity and the local source function as a quasi-invariant iteration factor into the "local" coefficient b :

$$b = \int_{-\infty}^{\infty} \phi(\nu) d\nu \oint \left[p + \frac{I_U e^{-\Delta}}{S_L} k(\varphi) \right] \frac{d\hat{\Omega}}{4\pi}, \quad (7)$$

where $k(\varphi)$ can be either zero or unity. The optimum results regarding acceleration and stability are obtained when the iteration factor is used in the so-called "in-going" sweeps (i.e. $k = 1$ for $0 < \varphi < \pi$) following tightly the idea of the FBILI method developed for 1D RT problems. We named this iterative procedure "Sweep-by-sweep Implicit Lambda Iteration."

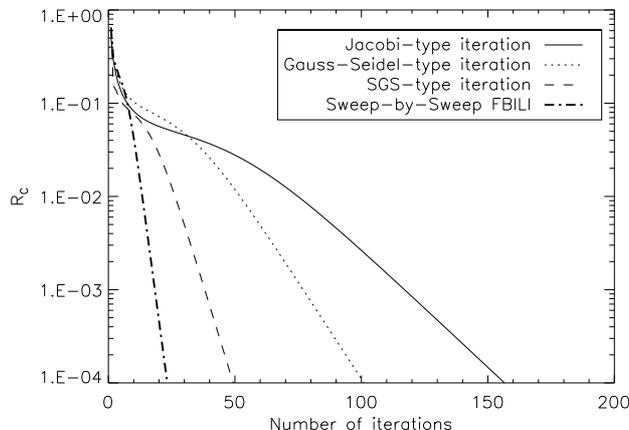


Figure 2: Evolution of the maximum relative change of S with iteration number for four described iterative procedures.

4. CONVERGENCE PROPERTIES

We tested the iterative procedures described above (Jacobi, Gauss-Seidel, Symmetric Gauss-Seidel, Sweep-by-sweep ILI) on a simple test problem given by Auer & Paleou (1994). They studied the two-level atom line transfer with complete frequency redistribution in a homogeneous and isothermal slab of dimensions $10^4 \times 10^4$. Planck function and opacity are equal to unity, and Gauss absorption-line profile is used. The slab is illuminated by the radiation field equal to unity from directions $\pi < \varphi < 2\pi$. For spatial discretization we use a 129×129 log-spaced grid.

In order to compare the convergence properties of various iterative procedures we computed and displayed the evolution of the maximum relative change of the source function between two successive iterations (R_c) with the number of iterations in Fig. 2.

It is obvious that each of the iterative procedures shows increase in the convergence rate with respect to the "previous" one. Let us note the amount of acceleration: Gauss-Seidel brings acceleration of about 70% with respect to the Jacobi iteration. It is somewhat less than in 1D case, which is the consequence of using comparatively lesser amount of new information in updating the source function (in 2D three out of four sweeps use the "old" source function values, while in 1D it happens in one out of the two sweeps). SGS is exactly two times faster than GS which is a significant improvement. Finally, the use of the iteration factor brings acceleration by more than a factor two with respect to SGS. In total, Sweep-by-sweep ILI is about 7 times faster than the state-of-the art Jacobi method, which is an improvement of almost an order of magnitude. More detailed analysis is given in Milić & Atanacković (2014), and additional test problem is studied in Milić (2014).

One of the properties of an iterative scheme which is of great importance in computations is its scaling with the grid resolution. Standard methods based on the approximate operator need more iterations to converge when the grid is refined. In 1D problems the total computing time of the Jacobi method scales with number of points like N^2 , where N is the resolution of the spatial grid, since both the computational work of the formal solver and the number of iterations needed to reach

Table 1: Number of iterations needed by the Jacobi and SsILI method to reach $R_C = 10^{-3}$ for various grid resolutions.

Grid resolution	33×33	65×65	129×129	257×257
Jacobi iteration	30	63	118	204
Sweep-by-sweep ILI	7	12	19	30

the convergence scale with N . We expect SsILI method to behave differently due to the use of the iteration factor (Eq. 7) as well. We solved the test problem described above with four different grid resolutions. Table 1 shows number of iterations that the Jacobi and SsILI method need to reach maximum relative change of 10^{-3} .

The results show that SsILI method scales better with the grid resolution than the Jacobi method. For example, the increase in resolution by a factor of 8 decreases the rate of convergence of the Jacobi method by a factor of almost 7, while that of the SsILI by less than a factor of 4 in order to reach $R_C = 10^{-3}$. In addition, it is important to keep in mind that, due to slower convergence rate, more strict convergence criterion than $R_C = 10^{-3}$ might be required for the Jacobi method to achieve the “exact” solution.

5. CONCLUSIONS

In this paper we briefly presented Sweep-by-sweep Implicit Lambda Iteration, a new iterative procedure for NLTE line radiative transfer on 2D Cartesian grids. As an intermediate step, we have also generalized Symmetric Gauss-Seidel method into 2D geometry. Sweep-by-sweep ILI significantly outperforms the existing methods, at least in this simple test problem. Our next steps will be the analysis of its convergence properties on inhomogeneous models, modeling of realistic lines using multilevel atom models and application of this method to NLTE modeling of scattering polarization in spectral lines.

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