Solution of NLTE Radiative Transfer Problems Using Forth-and-Back Implicit Lambda Iteration

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Abstract.   The basic idea of an extremely fast convergent iterative method, the Forth-and-Back Implicit Lambda Iteration, is briefly described and the applications of the method to various radiative transfer problems are listed and discussed.

1.   Introduction

Radiative transfer (RT) is the underlying physical phenomenon in many astrophysical problems and among the most difficult to deal with. The main difficulty arises from the non-local and in general non-linear coupling of the radiation field and the state of the gas.

In the problem of NLTE (non-local thermodynamic equilibrium) line formation in a given atmospheric model, the internal state of the gas depends, via radiative transitions, on the radiation field intensity, which in turn depends, via the RT process, on the state of the gas over a wide range of distant points. Mathematically, the non-local coupling is performed by the simultaneous solution of the corresponding RT equation describing the dependence of the mean intensity on the source function $J = \Lambda[S]$ by means of the so-called Λ operator and the statistical equilibrium (SE) equations defining the source function in terms of the mean intensity of the radiation field $S = S(J)$.

In the two-level-atom line formation problem the non-local coupling is linear and the problem can be easily solved by using either direct or iterative methods. In a more general multilevel case, RT problem is non-linear and, therefore, an iterative method is required.

The most straightforward iterative procedure, the so–called Λ iteration, solves radiative transfer and statistical equilibrium equations in turn. However, in most cases of interest (in scattering dominated media of large optical thickness) its rate of convergence is infinitely slow (Mihalas 1978).

A broad class of ALI (Approximate (or Accelerated) Lambda Iteration) methods, currently in use, is based on the use of certain physical or computational approximations of the Λ operator within an iterative procedure. These methods usually employ some free parameter controlling the convergence and almost always need additional acceleration by some mathematical techniques (Ng acceleration, successive over-relaxation method, etc.) to achieve high convergence rate (Hubeny 2003; Atanacković-Vukmanović 2004).

Atanacković-Vukmanović, Crivellari, & Simonneau (1997) developed the Forth-and-Back Implicit Lambda Iteration (FBILI) - a simple, accurate and

extremely fast convergent method to solve NLTE RT problems. FBILI dramatically accelerates the convergence of the classical Λ iteration while retaining its straightforwardness. In this paper the basic idea of the method is briefly explained and the applications to various RT problems are shown and discussed.

2. The Idea of FBILI Method

In order to demonstrate the basis of the FBILI method we shall consider the case of the two-level atom line formation (with complete redistribution and no overlapping continuum) in a plane-parallel and static atmosphere. Under these assumptions, the specific intensity of the radiation field $I_{x\mu}(\tau)$ is described by the RT equation of the form:

$$\mu \frac{dI_{x\mu}}{d\tau} = \varphi_x[I_{x\mu}(\tau) - S(\tau)] \quad , \tag{1}$$

where τ is the mean optical depth, x is the frequency displacement from the line center in Doppler width units, μ is the cosine of the angle between the photon's direction and the outward normal and φ_x is the absorption-line profile, normalized to unity. The line source function (SE equation for a two-level atom) has the following form:

$$S(\tau) = \varepsilon B(\tau) + (1 - \varepsilon)J_\varphi(\tau) \quad , \tag{2}$$

where ε is the standard NLTE parameter representing the branching ratio between the thermal (LTE) contribution $B(\tau)$ and the scattering term

$$J_\varphi(\tau) = \int J_x \varphi_x dx = \frac{1}{2} \int_{-1}^{1} d\mu \int_{-\infty}^{\infty} dx \varphi_x I_{x\mu}(\tau) \quad , \tag{3}$$

which accounts for the angle and frequency coupling of the specific intensities at the given depth point τ.

The basic idea of the forth-and-back implicit Λ iteration in the solution of the problem is as follows. First, as suggested by the existence of two separate boundary conditions, the FBILI uses a separate description of the propagation of the in-going intensities of the radiation field $I_{x\mu}^-(\tau)$ with initial conditions at the surface $(\tau = 0)$ and of the out-going intensities $I_{x\mu}^+(\tau)$ with initial conditions at the bottom of the atmosphere $(\tau = \tau_N)$. Second, although the values of the radiation field are unknown, its propagation can be easily represented by using the integral form of the RT equation and assuming polynomial (e.g. piecewise quadratic) representation of the source function between two successive depth points. Thus, for each depth point one can write linear relations for the specific intensities as functions of the unknown values of the source function and of its derivative. Following the idea of iteration factors, it is the iterative computation of the coefficients of these *implicit* relations (implicit, as the source function is a priori unknown), rather than that of the unknown functions themselves, which greatly accelerates the convergence of the direct iterative scheme.

In the first part of each iteration (forward process), proceeding from the upper boundary condition, using the integral form of the RT equation for the

in-going intensities for each layer (τ_{l-1}, τ_l):

$$I_{x\mu}^-(\tau_l) = I_{x\mu}^-(\tau_{l-1})e^{-\Delta\tau_l\varphi_x/\mu} + \int_{\tau_{l-1}}^{\tau_l} S(t)e^{-(\tau_l-t)\varphi_x/\mu}\frac{\varphi_x}{\mu}dt \quad , \tag{4}$$

where $\Delta\tau_l = \tau_l - \tau_{l-1}$, and assuming parabolic behavior for the source function $S'(\tau_{l-1})2(S(\tau_l) - S(\tau_{l-1}))/\Delta\tau_l - S'(\tau_l)$, one can write the linear *local implicit* relation

$$I_{x\mu}^-(\tau_l) = [\frac{a_{x\mu}^-}{S^o(\tau_l)} + b_{x\mu}^-]S(\tau_l) + c_{x\mu}^-S'(\tau_l) \ , \tag{5}$$

representing the values of the in-going intensities $I_{x\mu}^-(\tau_l)$ at a given optical depth point τ_l in terms of yet unknown values of the source function $S(\tau_l)$ and of its derivative $S'(\tau_l)$. Here, $a_{x\mu}^- I_{x\mu}^-(\tau_{l-1})e^{-\Delta\tau_l\varphi_x/\mu} + qS^o(\tau_{l-1})$ is computed with the old (known from the previous iteration) source function S^o, whereas $b_{x\mu}^-$ and $c_{x\mu}^-$ depend only on the known optical distance $\Delta\tau_l$. By integrating (5) over all frequencies and directions we obtain the linear relation

$$J_\varphi^-(\tau_l) = b_l^- S(\tau_l) + c_l^- S'(\tau_l) \tag{6}$$

representing *implicitly* the value of the in-going mean intensity. Thus, in the forward process, we differ from the classical Λ iteration that re-calculates J_φ^- from the old (known) source function $S^o(\tau)$, in using the old source function to compute, at each optical depth point $\tau_l(l = 1, N)$, the coefficients b_l^- and c_l^- of the linear relation (6). The coefficients are stored for further use in the backward process of computation of the new values of $S(\tau)$. Let us note here that the ratio in Eq. (5) of the non-local part of the in-going intensity $a_{x\mu}^-$ to the current source function $S^o(\tau_l)$ is actually the iteration factor. Since it is the only information that is carried from the previous iteration step, an extremely fast convergence is to be expected.

The final aim is to derive, at each optical depth point τ_l, an *implicit* linear relation between the 'full' mean intensity and the source function

$$J_\varphi(\tau_l) = a_l + b_l S(\tau_l) \tag{7}$$

that, together with equation (2), leads to the new source function. To obtain this, we need the coefficients of the corresponding relation for the out-going mean intensity.

In the backward process we proceed from the bottom where $I_{x\mu}^+(\tau_N)$, i.e. $J_\varphi^+(\tau_N)$ is known or more precisely, the coefficients of the *implicit* relation for the out-going specific intensities and, therefore, for the out-going mean intensity

$$J_\varphi^+(\tau_l) = a_l^+ + b_l^+ S(\tau_l) \quad , \tag{8}$$

are known at $\tau = \tau_N$. Eliminating $S'(\tau_N)$ from Eq. (6) (see Atanacković-Vukmanović et al. 1997) we obtain the linear implicit relation (7), which together with SE equation (2) leads to the new value of $S(\tau_N)$. The new values of $S(\tau_N)$, $S'(\tau_N)$ and, hence, $I_{x\mu}^+(\tau_N)$ are then used to compute the coefficients of the linear relation (8) in the next upper layer. Together with the coefficients of Eq.

(6) (stored in the forward process), we obtain the coefficients a_l and b_l of Eq. (7). The computation of a_l and b_l and the solution of Eq. (7) together with SE equation (2) to get a new source function $S(\tau_l)$ are performed during the backward process layer by layer to the surface. The process is iterated to the convergence.

3.   Applications of FBILI

The accuracy and efficiency of the FBILI method have been checked in several RT problems. Here, we list some of the applications.

3.1.   Two-level-atom line formation

The method was first developed for the two-level-atom line formation (with complete redistribution and no overlapping continuum) in a plane-parallel constant property medium (for details see Atanacković-Vukmanović 1991, Atanacković-Vukmanović et al. 1997). This case represents an ideal test for checking the numerical accuracy and stability of a new method. Namely, under such conditions the features of the solution depend only on the NLTE parameter ε that is usually very small, so that the numerical errors can easily blur the solution.

Thus, in order to test the stability of the method we solved the two-level atom problem with $\varepsilon = 10^{-12}$. The results are given in Fig. 1. They are compared with the exact discrete-ordinate solution (Avrett & Hummer 1965), obtained by using the same discretization in optical depth (10 points per decade). The asymptotic value of the maximum relative error of the order of 0.3% is reached already within 9-14 iterations. Namely, only nine iterations are sufficient for the maximum relative correction between two successive iterations (for all depth points) to be less than $\delta = 10^{-2}$ and 14 iterations for $\delta = 10^{-3}$. Hence, we see that a negligible additional effort (of the iterative computation of the coefficients of the *implicit* relations, instead of the mean intensities themselves) with respect to the classical Λ iteration results in an extremely fast convergence (about 10 FBILI iterations compared to about $1/\varepsilon$ classical Λ iterations, while one FBILI iteration takes only about 10% more CPU time than a classical Λ iteration).

In the literature the performances of various methods are usually given for $\varepsilon = 10^{-4}$. Thus, for this case, in Fig. 2 the convergence properties of the FBILI method are compared with those of the ALI methods that use diagonal and 3-diagonal approximate Λ^* operators (Hubeny 2003). Excellent convergence properties of the FBILI are evident. Using FBILI yields convergence that is comparable to or even faster (for $\delta \geq 10^{-3}$) than the 3-diagonal operator with Ng acceleration!

3.2.   Two-level-atom line formation: Partial redistribution

The FBILI method was applied to the case of the two-level atom line formation problem in which partial redistribution is taken into account in the paper by Atanacković-Vukmanović et al. (1997). The results reproduced the well-known ones by Hummer (1969). For the cases $\varepsilon = 10^{-4}$ and $\varepsilon = 10^{-8}$, 13 and 15 iterations, respectively, are enough to fulfill the criterion $\delta = 10^{-3}$ for all the frequencies and all optical depths.
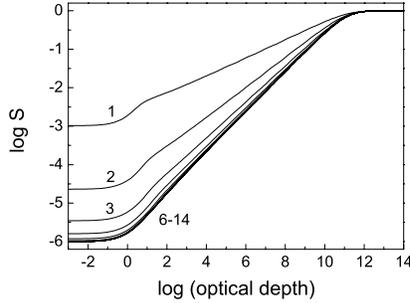
Figure 1.   Evolution with iterations of the source function for a two-level atom with $\varepsilon = 10^{-12}$ and $B = 1$.
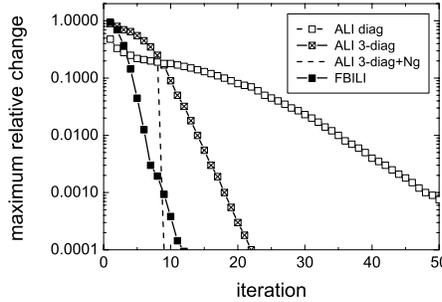

Figure 2.   Maximum relative change δ of the source function as a function of the iteration number, for different variants of the ALI scheme (reproduced from Fig. 1 in Hubeny 2003) and for the FBILI method. In all cases, two-level atom without continuum is considered, with $\varepsilon = 10^{-4}$, $B = 1$ and 4 depth-points per decade of optical depth.

3.3.   Multilevel-atom line formation

The procedure for multilevel problem is the same as in the two-level-atom case. Starting with the known set of level populations, we repeat the entire forward process for each radiative transition $i \rightarrow j$. In the backward process, layer by layer, we compute the coefficients of the linear relation (7) for all the transitions, and replacing them in the SE equations we solve the latter for the new set of level populations. The test is performed by solving the same problem (three-level hydrogen atom line formation in an isothermal atmosphere) as in Avrett & Loeser (1987). The solution with a maximum relative error below 3% is obtained in only nine iterations with the convergence criterion $\delta = 10^{-3}$ (see Atanacković-Vukmanović et al. 1997).

3.4.   Spherical radiative transfer: Monochromatic scattering

The generalization of the FBILI method to spherical geometry is performed by Atanacković-Vukmanović (2003). Monochromatic scattering problem in a

spherical atmosphere is solved and the results are compared with those given by Gros, Crivellari, & Simonneau (1997) and Avrett & Loeser (1984). The relative difference of the solutions is about 1%. The solution is obtained already in the second iteration, whereas three iterations are required for the maximum relative correction to be less than 1%.

3.5. Spherical radiative transfer: Line formation

In order to test the feasibility of the method when applied to the line formation in spherically symmetric media, the test problem of the line transfer with background absorption, proposed by Mihalas, Kunasz, & Hummer (1975) and Avrett & Loeser (1987), is solved. The solution is obtained in 15 iterations with an error less than 2%.

4. Conclusions

Forth-and-Back Implicit Lambda Iteration method is a simple, stable and extremely fast convergent iterative method developed for the exact solution of NLTE RT problems. A negligible additional computational effort with respect to the classical Λ iteration results in an extremely fast convergence. No additional acceleration is needed. The method is easy to apply. No matrix formalism is required so that the memory storage grows linearly with dimension of the problem. Due to its great simplicity and considerable savings in computational time and memory storage FBILI seems to be a far-reaching tool to deal with more complex problems (multidimensional RT, RT in moving media, or when RT has to be coupled with other physical phenomena).

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