Accelerated Lambda Iteration: An Overview

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Abstract. A brief review of the Accelerated Lambda Iteration (ALI) methods is presented. Besides explaining the basis of the method, three particular topics that are important for practical applications are discussed – construction of approximate Λ^* operators; efficient numerical methods for formal solution of the transfer equation; and the basic philosophy of applying the method beyond the simple case of two-level atom.

1. Introduction

Accelerated Lambda Iteration (ALI) is a simple yet very powerful numerical scheme that has revolutionized the field of stellar atmospheres and radiative transfer. As will be shown in many contributions in this Proceedings, we are now able to construct models of stellar atmospheres and other radiation-dominated objects (e.g., accretion disks, H II regions, etc.) with an unprecedented degree of realism and complexity. This was made possible both by the amazing development of computer capabilities, as well as by more efficient numerical methods, above all by ALI. It is thus quite appropriate to devote one of the introductory papers of this volume to this method.

2. The Problem

Let us demonstrate the basis of the problem with the following simple case, namely radiative transfer in a gas of two-level atom in a 1-D homogeneous, static medium. The problem consists of solving simultaneously two basic equations. The first one is the radiative transfer equation, written as

$$\mu \frac{dI_{\mu\nu}}{d\tau_{\nu}} = I_{\mu\nu} - S_{\nu} \,, \tag{1}$$

where $I_{\mu\nu}$ is the specific intensity of radiation, and S_{ν} the source function. The specific intensity depends on three variables, the frequency ν , the directional cosine μ , and the (monochromatic) optical depth τ_{ν} . Let us further assume no overlapping continuum and complete frequency redistribution (CRD), in which case the source function is independent of frequency, $S_{\nu} \equiv S$ (relaxing both approximations will be outlined in § 8.). The formal solution of (1) may be written as

$$I_{\mu\nu} = \Lambda_{\mu\nu}[S_{\nu}], \qquad (2)$$

where Λ operates on the quantity within the square brackets. By integration we obtain analogous relations for angle- and frequency-averaged quantities, viz.

$$J_{\nu} = \Lambda_{\nu}[S], \text{ where } J_{\nu} = \frac{1}{2} \int_{-1}^{1} I_{\mu\nu} d\mu \text{ and } \Lambda_{\nu} = \frac{1}{2} \int_{-1}^{1} \Lambda_{\mu\nu} d\mu,$$
 (3)

and

$$\bar{J} = \Lambda[S], \quad \text{where} \quad \bar{J} = \int J_{\nu} \phi_{\nu} d\nu \quad \text{and} \quad \Lambda = \int \Lambda_{\nu} \phi_{\nu} d\nu \,,$$
 (4)

where ϕ_{ν} the (normalized) absorption profile. J_{ν} and \bar{J} are mean intensity and frequency-averaged mean intensity, respectively. Analogously, we call Λ_{ν} and Λ the angle-averaged, and frequency- and angle-averaged Λ operator, respectively. For notational simplicity, we omit a bar on Λ .

The second basic equation is the equation of statistical equilibrium, which for a two-level atom may be written as an expression for the line source function,

$$S = (1 - \epsilon) \, \bar{J} + \epsilon B \,, \tag{5}$$

where ϵ is the collisional destruction probability, and B the Planck function. Substituting equation (4) into (5), we obtain a single integral equation,

$$S = (1 - \epsilon) \Lambda[S] + \epsilon B. \tag{6}$$

Because Λ is a linear operator, Eq. (6) may in fact be solved in a single step (but notice, this applies only for a two-level atom!). The solution can be formally written as

$$S = [1 - (1 - \epsilon)\Lambda]^{-1} [\epsilon B]. \tag{7}$$

However, due to the above-mentioned angle-frequency coupling, the matrix representing Λ may be large, so that inverting it may be quite time consuming, and therefore a direct solution may be impractical. This is why we seek faster, iterative, schemes.

We stress that in actual applications the Λ operator does not have to be constructed explicitly, nor does it have to be numerically inverted. By the terms "setting up" and "inverting" Λ operator we mean any procedure that solves the radiative transfer equation, together with equation(s) that specify the source function.

3. Ordinary and Accelerated Lambda Iteration

The simplest possibility is to iterate between the intensity and the source function; that is to evaluate the source function from equation (5) using the current specific intensity, and then to solve the transfer equation (1) or (2) using the new source function. This procedure is called "Lambda iteration". Specifically,

$$S^{(n+1)} = (1 - \epsilon)\Lambda[S^{(n)}] + \epsilon B. \tag{8}$$

This method is very simple. It treats all the coupling iteratively, so it avoids the need to invert the Lambda operator (matrix) completely. However, it is well known that it converges extremely slowly – see, e.g., Mihalas (1978); for a

very illustrative example, see Auer (1991; his Fig.1). And, worse yet, it exhibits a pathological behavior in that the solution *stabilizes* (i.e., relative changes of the source function become extremely small) long before the correct solution is reached.

More efficient iterative methods to handle these types of problems iteratively date back to the mid-nineteenth century, to the work of Jacobi. The first who applied the idea in the context of astrophysical radiative transfer was Cannon (1973), who in this seminal paper introduced the method of deferred corrections, also called, somewhat inaccurately, operator splitting. The idea consists of writing

$$\Lambda = \Lambda^* + (\Lambda - \Lambda^*), \tag{9}$$

where Λ^* is an appropriately chosen approximate lambda operator. The iteration scheme for solving Eq. (6) may then be written as

$$S^{(n+1)} = (1 - \epsilon)\Lambda^*[S^{(n+1)}] + (1 - \epsilon)(\Lambda - \Lambda^*)[S^{(n)}] + \epsilon B.$$
 (10)

The action of the exact Λ operator is thus split into two contributions: an approximate Λ^* operator that acts on the *new* iterate of the source function, and the difference between the exact and approximate operator, $\Lambda - \Lambda^*$, acting on the previous, *old* and thus known, source function. The latter contribution may be easily evaluated by the formal solution.

We emphasize that although we use an approximate operator, equation (6) is solved exactly, i.e., it is iterated to convergence, hence it is exact at the converged limit. If we choose $\Lambda^* = 0$, we recover the ordinary lambda iteration. On the other hand, the choice $\Lambda^* = \Lambda$ represents the exact method, which can be done without iteration, but an inversion of the exact Λ operator may be costly. Thus, in order that Λ^* brings an essential improvement over both methods, it has to incorporate all the essential properties of the exact Λ operator (in order to obtain a fast convergence rate of the iteration process), but at the same time it must be easy (and cheap) to invert. Therefore, the construction of the optimum Λ^* is a delicate matter. Cannon (1973) used a special variant of the Λ^* operator (angular and/or frequency quadratures of a low order) so that the advantages of the ALI method were not fully realized by most workers in the field. This realization came about a decade later, when Scharmer (1981) has reformulated an idea of ALI in a more physical way, and motivated an intensive development of the ALI-based approaches. The period of early development of the ALI method culminated in a seminal paper of Olson, Auer, & Buchler (1986) - OAB). We will return to construction of the Λ^* operator in Sect. 4.

We may write equation (10) in a slightly different form. First, we introduce an "intermediate" source function, namely that obtained from the old source function by the mere formal solution,

$$S^{\text{FS}} = (1 - \epsilon)\Lambda[S^{(n)}] + \epsilon B. \tag{11}$$

(superscript FS stands for "Formal Solution"). Using this definition, equation (10) can be rewritten as

$$\delta S^{(n)} \equiv S^{(n+1)} - S^{(n)} = [1 - (1 - \epsilon)\Lambda^*]^{-1} [S^{FS} - S^{(n)}].$$
 (12)

This equation is particularly instructive. To put it in a better perspective, let us rewrite the equation (8) that governs the traditional Lambda iteration, using equation (11),

$$\delta S^{(n)} = S^{FS} - S^{(n)}. \tag{13}$$

These equations show that the ALI iteration process is driven, similarly to ordinary Lambda iteration, by the difference between the old source function and the newer source function obtained by formal solution. However, unlike the ordinary Lambda iteration, this difference is *amplified* by the "acceleration operator", $[1 - (1 - \epsilon)\Lambda^*]^{-1}$.

To gain more insight, let us consider a diagonal (i.e., local) Λ^* operator. The appropriate Λ^* has to be chosen such that $\Lambda^*(\tau) \to 1$ for large τ (roughly speaking, because $I_{\nu} \to S_{\nu}$ for large τ). Because in typical cases $\epsilon \ll 1$, the acceleration operator indeed acts as a large amplification factor. This interpretation was first introduced by Hamann (1985) and Werner & Husfeld (1985), who also coined the term "Accelerated Lambda Iteration" (ALI). The acronym ALI is also sometimes understood to mean "Approximate Lambda Iteration".

Equation (12) can be also derived using a slightly different, but related, reasoning. Let us assume that we have a current estimate of the source function, S_0 . We write the correct source function as $S = S_0 + \delta S$. We further write the exact Λ operator as $\Lambda = \Lambda^* + \delta \Lambda$, i.e. as an approximate operator Λ^* plus a "perturbation" $\delta \Lambda$. We require that the source function satisfies equation (6), $S = (1 - \epsilon)\Lambda[S] + \epsilon B$. By substituting the perturbation expansions for S and Λ we obtain

$$S_0 + \delta S = (1 - \epsilon) \Lambda^* [S_0] + (1 - \epsilon) \Lambda^* [\delta S] + (1 - \epsilon) \delta \Lambda [S_0] + \epsilon B,$$

where we dropped the second-order contribution $\delta\Lambda[\delta S]$. By rearranging the terms we obtain

$$[1 - (1 - \epsilon)\Lambda^*][\delta S] = (1 - \epsilon)\Lambda[S_0] + \epsilon B - S_0 \equiv S^{FS} - S_0,$$
 (14)

where we used equation (11). Equation (14) is easily seen to be equivalent to equation (12). This procedure explains why the approach is sometimes called the "Operator Perturbation" method.

The ALI iteration scheme thus proceeds as follows:

- (a) For a given $S^{(n)}$ (with the initial estimate $S^{(0)} = B$, or some other suitable value), we perform a formal solution, for one frequency and angle at a time. We obtain new values of the specific intensity $I_{\mu\nu}$.
- (b) We calculate the new source function $S^{\rm FS}$ from equations (11), (3), and (4), using the new values of the specific intensity.
- (c) We then apply equation (12) to evaluate a new iterate of the source function, $S^{(n+1)}$.
- (d) Because the source function found in step (c) differs from that used in step (a), we iterate steps (a) through (c) to convergence.

To apply this idea efficiently in astrophysical radiative transfer problems, the following three issues are crucial: (i) evaluation of the optimum Λ^* operator; (ii) development of efficient, fast and accurate, formal solvers; and (iii) understanding how to go beyond simple academic case of two level atom.

4. Construction of the Λ^* Operator

4.1. Overview

Construction of the optimum approximate Λ -operator lies at the very heart of the method. As pointed out above, it has to satisfy two dichotomous conditions, namely it should be easy and cheap to invert, and it has to describe well the basic physics of the problem. Again, by the terms "constructing" and "inverting" the Λ^* operator we generally understand a *process* of solving the transfer equation in some approximate, though judicious, way.

We will not discuss here all possible variants of Λ^* operator; the interested reader is referred to Hubeny (1992) for the history of early development of the ALI method and a comprehensive list of references. We discuss only those forms that have survived the test of time, and which are being presently used in actual applications. There are several categories of the Λ^* operator, each category offers certain advantages and suffers from certain drawbacks.

4.2. Diagonal Operators

In one of the seminal papers on astrophysical radiative transfer, Olson, Auer, & Buchler (1976) showed that a nearly optimum Λ^* operator is in fact the diagonal part of the exact Λ operator,

$$\Lambda^* = \Lambda^*(\tau) \mathbf{I}, \tag{15}$$

where I is the unit diagonal matrix, and we understand $\Lambda^*(\tau)$ as a simple scalar function of τ . This variant of ALI is sometimes called the Jacobi method (e.g., Trujillo Bueno & Fabiani Bendicho 1995). A diagonal operator is indeed the easiest one to use because its inversion is a simple scalar division. However, how does one evaluate the diagonal part of exact Λ efficiently? There are several possibilities, depending on exactly which formal solver of the transfer equation is used.

• Quite generally, the diagonal part can be evaluated as

$$\Lambda_{dd} = \Lambda[\delta(\tau_d - \tau)]. \tag{16}$$

In other words, the diagonal element of the Λ matrix at depth point d is equal to the mean intensity (or the specific intensity, in the case of elementary, frequency-and angle-dependent $\Lambda_{\mu\nu}$) computed for the source function having a zero value everywhere but at the point d, i.e., $S_d = 1$, and $S_i = 0$, $(i \neq d)$. As follows from equation (16), to evaluate the diagonal operator at τ_d , we merely have to take the coefficient that multiplies $S(\tau_d)$. This method can be used with many formal solvers, including the short characteristics method (in one or more dimensions), or the Discontinuous Finite Element Method (Castor et al. 1992).

• Olson & Kunasz (1987) were the first to suggest applying the method of short characteristics to evaluate the Λ^* operator. In this case, one can either use the approach from the previous item, or one can also write down explicit expressions for Λ^* . For instance, using the linear form of the short characteristics method, one obtains for the approximate operator corresponding to the mean intensity of radiation, Λ^*_{ν} , namely

$$\Lambda_{\nu}^{*} = 1 - \frac{1}{2} \int_{0}^{1} \left(\frac{1 - e^{-\Delta \tau_{d-1/2}}}{\Delta \tau_{d-1/2}} + \frac{1 - e^{-\Delta \tau_{d+1/2}}}{\Delta \tau_{d+1/2}} \right) d\mu.$$
 (17)

where $\Delta \tau_{d-1/2} = \tau_d - \tau_{d-1}$ and analogously for $\Delta \tau_{d+1/2}$.

• Rybicki & Hummer (1991) used a formalism based on the Feautrier scheme, employing a very efficient and clever algorithm for inverting a tridiagonal matrix, and demonstrated that the entire set of the diagonal elements of Λ can be found with an order of ND operations (ND being the number of depth points). Thus, if one uses the Feautrier method as a formal solver, the Rybicki-Hummer method of evaluation of Λ^* is the method of choice.

A drawback of the diagonal operator is that the convergence speed decreases with increasing spatial resolution, which was first demonstrated by OAB. In other words, the higher the depth resolution, the lower the convergence speed. This is easily understood. Roughly speaking, in a finer grid, the information must go through more points in order to propagate the same distance in the optical depth space, and therefore the iteration is slower. However, in many applications one needs high spatial resolution. A possible cure is an application of the multigrid methods (Steiner 1991; Trujillo Bueno & Fabiani Bendicho 1995).

4.3. Higher Multi-Band Operators

Olson & Kunasz (1987) suggested the use of a tridiagonal part of the exact Λ -operator as an even better approximate Λ^* operator. They presented expressions for off-diagonal elements based on the short characteristic method, which are analogous to, but more complicated than, equation (17). The off-diagonal elements may also be easily evaluated in the context of the Rybicki-Hummer scheme.

Analogously, one may use an even higher multi-band part of the exact Λ operator. As can be expected, using penta-diagonal and higher-order multi-band operators will increase a speed of convergence, but this gain is somewhat outweighed by increasing numerical work to evaluate the corresponding matrix elements. A systematic study of the effects of the number of bands on the properties of the ALI iteration process was undertaken by Hauschildt (1992),.

4.4. Gauss-Seidel Approximate Operator

In a very interesting and important paper, Trujillo Bueno & Fabiani Bendicho (1995) suggested a different form of the Λ^* operator, namely an upper-triangular part of the exact Λ operator. Notice that already Scharmer (1981) suggested using an upper-triangular form of Λ^* , namely that based on a generalized Eddington-Barbier relation. His operator was thus inherently approximate.

Although evaluating an upper triangular part of the exact Λ is non-trivial, they suggested an ingenious procedure to set up and invert the upper triangular Λ^* operator, in the context of the short characteristic method, with essentially the same computational effort as with the diagonal Λ^* .

4.5. Practical Considerations

Experience shows that for most applications, using a diagonal Λ^* operator is a safe bet. Moreover, it is the only practical choice for multi-dimensional geometries. Although tridiagonal or higher-order band operators yield faster convergence for 1-D problems, their application for multilevel transfer problems is more difficult, and sometimes the gain in a lowered number of iterations is somewhat offset by the increased numerical work needed in setting up necessary quantities.

5. Formal Solvers

By the term *formal solution* we understand a numerical solution of the transfer equation in the case where the source function is fully specified. As explained above, the ALI method essentially reduces the general transfer problem into a set of formal solutions. This means that the speed with which we solve a general problem is largely determined by the speed of the formal solution. Therefore, we have to seek as efficient numerical schemes for performing a formal solution as possible.

There are essentially two classes of methods, namely those based on the first-order form of the transfer equation, and those based on the second-order form. The most important first-order methods are the method of short characteristics, and the discontinuous finite-element (DFE) method. The second-order method is usually referred to as the Feautrier method, after its originator (Feautrier 1964), although the general idea was first suggested in a seminal paper by Schuster (1905; see also Mihalas 1999)

5.1. Method of Short Characteristics

We describe the method here as applied for 1-D problem; its full strength lies in its application in multi-dimensional problems, discussed elsewhere in this volume.

The idea is to divide the medium into a number of cells, and to write down a simple formal solution of the transfer equation within the cell, assuming that the source function within the cell is approximated by a simple polynomial (linear or quadratic). Consider a given frequency ν along a ray at angle-cosine μ ; we shall drop explicit indication of frequency and angle variables. Denote the the monochromatic optical depth at this frequency along this ray as τ

The formal solution within the cell is written by (adopting the convention that the optical depth decreases in the direction of photon propagation)

$$I(\tau_d) = I(\tau_{d+1})e^{-\Delta\tau_{d+1/2}} + \int_{\tau_d}^{\tau_{d+1}} S(t) e^{-(t-\tau_d)} dt, \qquad (18)$$

If we assume that S is given by a linear or quadratic polynomial, the integral in equation (18) can be evaluated analytically, and the intensity at point τ_d can

be written as

$$I(\tau_d) = I(\tau_{d+1})e^{-\Delta\tau_{d+1/2}} + \lambda_{d,d-1}^+ S(\tau_{d-1}) + \lambda_{d,d}^+ S(\tau_d) + \lambda_{d,d+1}^+ S(\tau_{d+1}), \quad (19)$$

where the actual form of coefficients λ depends on whether one uses linear of quadratic representation of the source function. Detailed expressions for these quantities are given by Olson & Kunasz (1987). In the linear case, $\lambda_{d,d-1}^+ = 0$. In equation (19), the boundary value of the specific intensity, $I(\tau_{d+1})$ is given either by the boundary conditions of the problem (if the point d+1 is at the boundary), or by the outgoing intensity from the previous cell between d+2 and d+1. One thus proceeds from the boundary where the incoming radiation is specified to the other boundary.

5.2. Discontinuous Finite-Element Method

The method was was introduced by Castor, Dykema, & Klein (1992), and is essentially an application of the Galerkin method. An idea is again to divide a medium into a set of cells, and to represent the source function within a cell by a simple polynomial, in this case by a linear segment. Unlike the short characteristics method, the segments are assumed to have step discontinuities at grid points. The specific intensity at grid point d is thus characterized by two values I_d^+ and I_d^- appropriate for cells (τ_d, τ_{d+1}) and (τ_{d-1}, τ_d) , respectively (notice that we are dealing with an intensity in a given direction; the superscripts "+" and "–" thus do not denote intensities in opposite directions as it is usually used in the radiative transfer theory). The actual value of the specific intensity $I(\tau_d)$ is given as an appropriate linear combination of I_d^+ and I_d^- . We skip all details here; suffice to say that after some algebra one obtains simple recurrence relations for I_d^+ and I_d^-

$$a_d I_d^- - 2I_{d+1}^- = \Delta \tau_{d+1/2} S_{d+1} + b_d S_d, \qquad (20)$$

$$a_d I_{d+1}^+ = 2(\Delta \tau_{d+1/2} + 1) I_{d+1}^- + b_d S_{d+1} - \Delta \tau_{d+1/2} S_d.$$
 (21)

As was shown by Castor et al., the method is second-order accurate. Since one does not need to evaluate any exponentials, the method is usually the fastest formal solution.

5.3. Feautrier Method

The method and its extensions was described many times in the literature (Feautrier 1964; Auer 1976; Mihalas 1978; Rybicki & Hummer 1991), so there is no need to go to any details here. We just outline the basic features. The method consists in introducing the symmetric and antisymmetric parts of the specific intensity (assuming $\mu > 0$).

$$j_{\mu\nu} = [I(+\mu,\nu) + I(-\mu,\nu)]/2$$
, and $h_{\mu\nu} = [I(+\mu,\nu) - I(-\mu,\nu)]/2$, (22)

which have, respectively, a mean-intensity-like and flux-like character. Adding and subtracting these equations one obtains first-order differential equations for j and h, (assuming here a source function independent of direction),

$$\mu(dh_{\mu\nu}/d\tau_{\nu}) = j_{\mu\nu} - S_{\nu} , \qquad (23)$$

$$\mu(dj_{\mu\nu}/d\tau_{\nu}) = h_{\mu\nu} . \tag{24}$$

Eliminating $h_{\mu\nu}$, one obtains a second-order equation for $j_{\mu\nu}$,

$$\mu^2(d^2j_{\mu\nu}/d\tau_{\nu}^2) = j_{\mu\nu} - S_{\nu}. \tag{25}$$

We stress that S_{ν} is assumed to be fully specified. We can thus solve equation (25) for one frequency-angle point at a time. For simplicity, we drop indices μ and ν . By discretizing, and adding appropriate boundary conditions, one arrives at a tridiagonal system, written formally as

$$-A_d j_{d-1} + B_d j_d - C_d j_{d+1} = \tilde{S}_d, \quad \text{with} \quad A_1 = C_{ND} = 0, \tag{26}$$

where d is the depth index; \tilde{S}_d is a quantity which is equal to the source function everywhere but at the boundary points d=1 and d=ND where one has contributions from the incoming radiation intensities. Equation (26) is solved by a standard Gaussian elimination, consisting of a forward-backward recursive sweep.

5.4. Electron Scattering

To avoid misunderstanding, we stress that by the term formal solution one sometimes understands a solution for one frequency at a time, with given *thermal* source function. The total source function is given by

$$S_{\nu} = S_{\nu}^{\text{therm}} + \frac{n_{\text{e}}\sigma_{\text{e}}}{\chi_{\nu}} J_{\nu} , \qquad (27)$$

where the last term describes the electron (Thomson) scattering, assumed here to be strictly coherent. In this case, the total source function is not fully specified, but depends on J_{ν} even in the "formal" solution.

There are three possibilities to cope with this problem:

- i) Using a Λ -iteration procedure. We replace unknown J_{ν} in Eq. (27) by the current value J_{ν}^{old} , use any of the methods described previously to obtain new $I_{\mu\nu}$ and J_{ν} , and iterate. If the electron scattering is not a dominant contribution to the total source function, the procedure converges quite fast.
- ii) One may use the ALI procedure. This is completely analogous to the case of two-level atom discussed above. Since we consider a given frequency, the only coupling is the angular one. Formally, in equation (5), ϵB is replaced by $S_{\nu}^{\rm therm}$, $(1-\epsilon)$ by $n_{\rm e}\sigma_{\rm e}/\chi_{\nu}$, and \bar{J} by J_{ν} . The problem is thus reduced to a set of true formal solutions for one frequency and angle at a time, and any of the above methods may be used.
- iii) When using the Feautrier method, one may treat the angular coupling that arises due to electron scattering directly. To this end, one introduces vector $\mathbf{sj_d} = (j_{d,1}, \ldots, j_{d,NA})$, where NA is the number of angle points (we dropped the frequency index). We then apply equation (26), where A, B, C are now $NA \times NA$ matrices, and \mathbf{j}_d and \mathbf{S}_d vectors of length NA. For details refer, e.g., to Mihalas (1978).

6. Acceleration of Convergence

It is well known from linear algebra that any iterative method which evaluates the next iterate using solely the current iterate may converge at best linearly. However, taking into account information from previous iterates, one may estimate an extrapolated iterate, and the overall iteration scheme may be significantly faster. In the context of astrophysical radiative transfer, the idea was first used by Hamann (1981) who applied the Aitken extrapolation scheme to accelerate the ordinary Lambda iteration. At present, two most powerful schemes are the Ng acceleration (Ng 1974; OAB; Auer 1987; Hubeny & Lanz 1992)— also called the residual minimization technique; and the orthogonal minimization technique — Orthomin (Klein et al. 1989; Auer 1991).

The most widely used scheme is the Ng acceleration. A general expression for the accelerated estimate of the solution in the n-th iteration is

$$\mathbf{x}^{\text{acc}} = \left(1 - \sum_{m=1}^{M} \alpha_m\right) \mathbf{x}^{(n)} + \sum_{m=1}^{M} \alpha_m \mathbf{x}^{(n-m)}, \qquad (28)$$

where the coefficients α are determined by residual minimization; \mathbf{x} denotes the vector of unknowns (e.g., in the case of two-level atom, the vector of source functions at all depths). In most applications one uses M=2, i.e. an accelerated estimated is computed using the current and two previous iterates. There are two other practical issues, namely at which point in the sequence of iterations to perform the acceleration for the first time, and what interval to use between subsequent accelerations. Experience shows that it is usually advisable to wait for a certain number of iterations before performing the first acceleration – in the case of two level atom an optimum value is close to 7, i.e. one performs the first acceleration at the 7-th iteration. Also, although the accelerated solution vector can be calculated after each iteration, it is more efficient to perform an acceleration every, say, 4-6 iterations.

Here we also mention the method of successive over-relaxation (SOR), has been applied in the context of ALI by Trujillo Bueno & Fabiani Bendicho (1995). Although, strictly speaking, it is not a genuine acceleration method, it uses the idea of enhancing the current iteration correction using information from the previous iterates. Roughly speaking, instead of using the correction δS which follows directly from the ALI method [e.g., from equation (14)], one computes the new source function as $S^{\text{new}} = S^{\text{old}} + \alpha \, \delta S$, where α is an over-relaxation coefficient. There are several possibilities for evaluating α ; a practical procedure suggested by Trujillo Bueno & Fabiani Bendicho is to express α in terms of the spectral radius of the appropriate iteration operator, which in turn is given as a ratio of maximum relative changes of the source function in two subsequent previous iterations.

7. Some Representative Numerical Results

In order to test the performance of different variants of the Λ^* operator and the effects of the acceleration techniques, we have computed a series of test examples. We display here representative results for the simple case of a two-level atom without continuum, i.e. with the source function given by equation

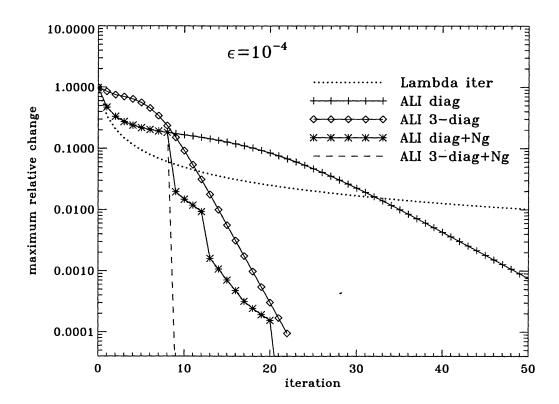


Figure 1. Maximum relative change of the source function as a function of the iteration number, for different variants of the ALI scheme. In all cases, we consider two-level atom without continuum, with depthindependent $\epsilon = 10^{-4}$ and B = 1. We assume 4 depth-points per decade of optical depth. Traditional Lambda iteration is shown for comparison.

(5), where we adopt $\epsilon \equiv 10^{-4}$ and $B \equiv 1$ independent of depth. The results are obtained by a pedagogically-oriented program ALIRTE, (Hubeny 1994), which will be provided to an interested user upon request.

Figure 1 illustrates the behavior of the ALI iteration process when using different variants of the Λ^* operator, together with the effects of the Ng acceleration. The simplest ALI variant, a diagonal Λ^* with no acceleration, converges relatively slowly, although still much faster than the traditional Lambda iteration. The tridiagonal operator yields much faster convergence. However, using Ng acceleration with a diagonal operator yields convergence that is comparable to or faster than the tridiagonal operator!

8. More Realistic Applications of ALI

The academic case of two-level atom without overlapping continuum is a pedagogical tool to demonstrate the basic features of line transfer, but reality is usually more complex. In this section, we outline the strategy of how to deal with more complicated situations.

Inspecting the case of two-level atom, one realizes that the ease with which the idea of ALI was applied follows from the fact that the radiation intensity enters the expression for the total source function only through a single frequency-and angle-integrated quantity, \bar{J} . So, here is the rule of thumb: in all the situations where this is not the case (we shall show some such situations below), the basic strategy is to find a quantity which is frequency- and angle-integrated, and through which the total source function can be expressed.

8.1. Two-level atom with continuum

The simplest such case is provided by the two-level atom with a background continuum. In this case the total source function is given by (Mihalas 1978)

$$S_{\nu}^{\text{tot}} = \frac{\phi_{\nu}}{\phi_{\nu} + r} S^{L} + \frac{r}{\phi_{\nu} + r} S^{C}$$
 (29)

where $S^{\rm L}$ is a frequency-independent line source function, given by equation (5); $S^{\rm C}$ is the source function in the continuum, and $r = \kappa^{\rm C}/\kappa^{\rm L}$ is the ratio of the continuum to the frequency-averaged line opacity. Both $S^{\rm C}$ and r are viewed as given.

Here the choice of the frequency- and angle-integrated quantity is obvious: it is the line source function. The specific intensity is expressed through the elementary lambda operator acting on the total source function,

$$I_{\mu\nu} = \Lambda_{\mu\nu} \left[S_{\nu}^{\text{tot}} \right] = \Lambda_{\mu\nu} \left[\frac{\phi_{\nu}}{\phi_{\nu} + r} S^{L} + \frac{r}{\phi_{\nu} + r} S^{C} \right]. \tag{30}$$

Substituting this to equation (5), we obtain for the line source function

$$S^{\mathcal{L}} = (1 - \epsilon) \Lambda [S^{\mathcal{L}}] + S_0, \qquad (31)$$

where

$$\Lambda[S] = \frac{1}{2} \int_{-1}^{1} d\mu \int_{0}^{\infty} \phi_{\nu} \Lambda_{\mu\nu} \left[\frac{\phi_{\nu}}{\phi_{\nu} + r} S \right] d\nu , \qquad (32)$$

and

$$S_0 = (1 - \epsilon) \frac{1}{2} \int_{-1}^1 d\mu \int_0^\infty \phi_\nu \Lambda_{\mu\nu} \left[\frac{r}{\phi_\nu + r} S^C \right] d\nu + \epsilon B, \qquad (33)$$

so that S_0 is a known function.

Equation (31) is analogous to the expression for the (line) source function without the background continuum. We may therefore use exactly the same iterative scheme as described above, where the only difference is that the integrated approximate Λ^* operator is given by an expression analogous to (32). In the case of diagonal approximate operator, $\bar{\Lambda}^*$ is a scalar function of τ , and is given by

$$\Lambda^*(\tau) = \frac{1}{2} \int_{-1}^1 d\mu \int_0^\infty \frac{\phi_\nu^2}{\phi_\nu + r} \, \Lambda_{\mu\nu}^*(\tau) \, d\nu \,. \tag{34}$$

8.2. A More Complex Example: Partial Redistribution

The case of partial redistribution (PRD) is discussed in detail elsewhere in this Proceedings (Nagendra; Uitenbroek). Here we consider only how one can apply ALI methods to such more complicated cases.

Source function for a two-level atom without assumption of complete frequency redistribution is generally given by

$$S_{\mu\nu} = \frac{\phi_{\nu}}{\phi_{\nu} + r} S_{\mu\nu}^{\text{PRD}} + \frac{r}{\phi_{\nu} + r} S^{\text{C}},$$
 (35)

where

$$S_{\mu\nu}^{\rm PRD} = (1 - \epsilon) \frac{1}{2} \int_{-1}^{1} d\mu' \int_{0}^{\infty} R(\nu', \mu', \nu, \mu) I_{\nu'\mu'} d\nu' + \epsilon B, \qquad (36)$$

where R is the redistribution function (Hummer 1962; Mihalas 1978). [Notice that many applications assume the isotropic approximation in which the source function is formulated through angle-averaged redistribution function $R(\nu', \nu)$. Here, we consider a full frequency- and angle-dependent redistribution function, and similarly for the source function.] Because the source function now depends explicitly on frequency and angle, there is no natural μ - and ν -integrated quantity here. However, the redistribution function satisfies the following normalization condition (assuming isotropic scattering – see Hummer 1962),

$$\frac{1}{2} \int_{-1}^{1} d\mu \int_{0}^{\infty} R(\nu', \mu', \nu, \mu) d\nu = \phi(\nu'), \qquad (37)$$

hence

$$\frac{1}{2} \int_{-1}^{1} d\mu \int_{0}^{\infty} S_{\mu\nu}^{PRD} d\nu = S^{L}.$$
 (38)

So, we may express $S_{\mu\nu}^{\rm PRD}$ as $S_{\mu\nu}^{\rm PRD}=a_{\mu\nu}\,S^{\rm L}$, and adopt $S^{\rm L}$ as the desired frequency- and angle-integrated quantity.

The numerical scheme proceeds as two nested iteration loops (first suggested by Scharmer 1983):

- estimate $a_{\mu\nu}$ (typically, initialize $a_{\mu\nu}=1$);
- hold $a_{\mu\nu}$ fixed, and iterate for $S^{\rm L}$ exactly as in the usual ALI treatment of CRD two-level atom with continuum;
 - after the inner loop is finished, update $a_{\mu\nu}$, and repeat.

8.3. Multilevel Atoms

This is the most important application of ALI in stellar atmospheric modeling. This topic will be discussed in more detail in a companion paper (Hubeny & Lanz; this volume), and in a number of other contributions in this Proceedings, so it will be not discussed here.

9. Conclusions

I have outlined here the basic principles of the Accelerated Lambda Iteration method. I have concentrated on three particular topics, construction of the approximate Λ^* operator, most efficient formal solvers, and the philosophy of applying ALI in more complicated cases.

Many of the subsequent papers of this Proceedings will discuss details of further extensions and applications of the ALI method, in particular to multilevel problems, polarized radiation, multi-dimensional geometries, etc. All these papers will demonstrate that the ALI method is indeed the true workhorse of the modern stellar atmospheres theory.

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