THE ASTROPHYSICAL JOURNAL, 455:646–657, 1995 December 20

A NOVEL ITERATIVE SCHEME FOR THE VERY FAST AND ACCURATE SOLUTION OF NON-LTE RADIATIVE TRANSFER PROBLEMS

J. TRUJILLO BUENO AND P. FABIANI BENDICHO[1]
Instituto de Astrofisica de Canarias, E-38200, La Laguna, Tenerife, Spain; jtb@iac.es
Received 1995 April 6; accepted 1995 June 27

ABSTRACT

Iterative schemes based on Gauss-Seidel (G-S) and *optimal* successive overrelaxation (SOR) iteration are shown to provide a dramatic increase in the speed with which non-LTE radiation transfer (RT) problems can be solved. The convergence rates of these new RT methods are identical to those of *upper* triangular *nonlocal* approximate operator splitting techniques, but the computing time per iteration and the memory requirements are similar to those of a *local* operator splitting method. In addition to these properties, both methods are particularly suitable for multidimensional geometry, since they neither require the actual construction of *nonlocal* approximate operators nor the application of any matrix inversion procedure.

Compared with the currently used Jacobi technique, which is based on the *optimal* local approximate operator (see Olson, Auer, & Buchler 1986), the G-S method presented here is faster by a factor 2. It gives excellent smoothing of the high-frequency error components, which makes it the iterative scheme of choice for *multigrid* radiative transfer. This G-S method can also be suitably combined with standard acceleration techniques to achieve even higher performance.

Although the convergence rate of the *optimal* SOR scheme developed here for solving non-LTE RT problems is much higher than G-S, the computing time per iteration is also minimal, i.e., virtually identical to that of a *local* operator splitting method. While the conventional *optimal* local operator scheme provides the converged solution after a total CPU time (measured in arbitrary units) approximately equal to the number n of points per decade of optical depth, the time needed by this new method based on the *optimal* SOR iterations is only $\sqrt{n}/2\sqrt{2}$. This method is competitive with those that result from combining the above-mentioned Jacobi and G-S schemes with the best acceleration techniques.

Contrary to what happens with the local operator splitting strategy currently in use, these novel methods remain effective even under extreme non-LTE conditions in very fine grids.

Subject headings: methods: numerical — radiative transfer — stars: atmospheres

1. INTRODUCTION

Advances in our understanding of stellar atmospheres (and of some other astrophysical systems) largely depend on our ability to develop very fast and accurate numerical radiative transfer (RT) methods. There are two main reasons for this. First, suitable diagnostic techniques can be developed to deduce, from the measurable properties of the radiation field, the chemical composition and the thermodynamic and dynamic state of astrophysical plasmas. Second, processes of energy and momentum exchange by radiation play an important role in the structure and dynamical behavior of many astrophysical fluids; consequently, it is often mandatory to couple the RT and the magnetohydrodynamic equations when trying to provide a suitable physical explanation of the observed phenomena. Over the last 10 years we have witnessed impressive progress in these two branches, driven in part by the application of a number of efficient iterative algorithms and powerful mathematical techniques (see, e.g., Auer, Fabiani Bendicho, & Trujillo Bueno 1994, and more references therein). However, as explained below, it is unlikely that the iterative algorithms currently in use will allow any further *dramatic* progress, except perhaps through the use of massively parallel computers. This paper aims at presenting a novel iterative scheme that allows RT problems to be solved with an order-of-magnitude improvement over the fastest methods currently in use.

During the last decade the literature on RT has been particularly abundant with respect to the mathematical techniques, which have become the methods of choice for the numerical solution of large-scale non-LTE problems in which there is nonlocal coupling due to *scattering*. These are the so-called accelerated (or approximated) Λ-iteration techniques, in which the symbol Λ is used to designate the operator that, acting on the source function, leads to the radiation intensity (see, e.g., the overviews given by Kalkofen 1987; Rybicki 1991; Hubeny 1992). These methods are based on the idea of "operator splitting" (Varga 1962; Cannon 1973), in which the discrepancy between the approximate and the exact operators is used to generate a correction to the previous estimate. The basic difference between the various strategies proposed lies in the choice of the approximate Λ-operator: if a *nonlocal* one is chosen, then spatial couplings are taken into account, and the computing time per iteration may be relatively large, given the need to construct the approximate operator and to perform matrix inversions, but the number of required iterations may be small; if a *local* one (i.e., diagonal) is chosen, the computing time per iteration is the smallest that can be achieved, but the number of required iterations may become relatively large.

The present state of the art in this context is basically the following. One may choose either the optimal *local* operator

[1] ESA fellow at the Kiepenheuer-Institut für Sonnenphysik, Schöneckstrasse 6, D-79104 Freiburg, Germany; pfb@kis.uni-freiburg.de.

given by the diagonal of the true Λ operator (see Olson, Auer & Buchler 1986, hereafter OAB), or select a *nonlocal* operator such as, for example, the one proposed by Scharmer (1981) or any of those *banded* operators that take into account spatial couplings with the neighbor points (Olson & Kunasz 1987). For example, with Scharmer's (1981) global operator, which is suitable for *one dimensional* applications *only*, one finds CPU time advantages with respect to the *optimal* local operator method (generally not larger than a factor 2) for few-level model atom configurations, while for many-level problems the optimal *local* operator choice combined with Ng's (1974) acceleration technique is faster, and the global operator quickly becomes prohibitive in its memory requirements (Carlsson 1991). On the contrary, taking only *nearest* neighbor depth couplings into account in one-dimensional situations leads to a tridiagonal system of equations, and the extra computing time per iteration is not substantial (see Olson & Kunasz 1987; see also, e.g., Rybicki & Hummer 1991). As shown in these references, the saving in the number of required iterations to reach convergence, which can be achieved by selecting such a one-dimensional tridiagonal operator instead of the optimal local one, is about a factor 2 when such operator splitting methods are combined with Ng's (1974) acceleration of convergence technique. However, in two and three dimensions an approximate operator that takes *nearest* neighbor couplings into account is very costly both to construct and to invert; for example, in two-dimensional Cartesian coordinates it leads to a system of equations with a tridiagonal augmented by two bands of width 3 separated from the main diagonal by a number of elements equal to the number of horizontal grid points, while the number of alternating zero and nonzero bands in three-dimensional situations is even larger (Kunasz & Olson 1988; Väth 1994). Therefore, in two and three dimensions, avoiding the *actual* construction and inversion of *nonlocal* operators is truly essential, while in one-dimensional situations the best approach at present is, in practice, either to use the optimal local approximate operator or the tridiagonal one, which typically leads to a CPU-time saving factor not larger than 2 for scalar class computers.

Another method of potential interest for RT applications (mainly for two- and three-dimensional problems) is the *multigrid* method (Hackbush 1985; Steiner 1991; Fabiani Bendicho, Trujillo Bueno, & Auer 1994). Each *multigrid* iteration is basically composed of two essential parts: a *smoothing* one, in which a few iterations in the desired *fine* grid using a suitable iterative scheme should get rid of the high-frequency components of the error of the current estimate, and the actual corrections evaluated by interpolating to the *fine* grid the solution of the error equation obtained in a *coarser* grid. For the *smoothing* part, both *local* and *nonlocal* splitting schemes have been used (see Steiner 1991), with the result that the optimal *local* operator method (which has the above-mentioned advantages) has a much worse smoothing capability than the nonlocal one, often leading to failure of the multigrid iteration.

It is clearly of great potential interest to develop a new general RT iterative scheme (equally applicable to one-dimensional and multidimensional geometries) with a convergence rate and a smoothing efficiency *identical* to that of a highly *nonlocal* operator splitting method, but with memory requirements and a computing time per iteration similar to those of the *local* operator method. In this paper we introduce such a novel iterative scheme and two new RT methods based on it, which lead to saving a remarkable amount of computational time with respect to the splitting methods discussed above. We concentrate here on considering *linear* RT problems, such as the coherent scattering or the two-level atom line transfer case. We have already applied the very same methods (developed below) to the multilevel atom case with successful results. However, for the sake of clarity with the present paper, we postpone the extension to the full *nonlinear* multilevel problem for a forthcoming publication (Trujillo Bueno & Fabiani Bendicho 1995), in which we shall show how the preconditioning strategy of Rybicki & Hummer (1991) can be suitably generalized to achieve such a goal.

The outline of this paper is as follows. Section 2 begins presenting (for the case of a linear system of equations) the general iterative scheme from which a number of basic iterative methods are obtained once the corresponding approximate operator is selected. One of these methods is the one proposed by Jacobi (1845), for which the approximate operator is the *optimal* local one. This was developed by OAB in a way suitable for RT applications. The other two iterative methods form the basis of the present paper; they are the Gauss-Seidel (G-S) and the successive overrelaxation (SOR) schemes (Seidel 1874; Young 1950), whose convergence properties are *identical* to those of upper (or lower) triangular splitting operator methods. In § 3 we describe how these methods can be applied efficiently to RT problems, i.e., we develop a technique based on the "short characteristics" formal solution strategy (Kunasz & Auer 1988; Auer & Paletou 1994; Auer et al. 1994), which allows us to perform G-S and SOR iterations at the same computational cost than that required by Jacobi's ones. This will allow us to clarify and emphasize that, in spite of the fact that our G-S and SOR RT methods have the high convergence rates of upper triangular operators, they neither require the actual calculation of such approximate *nonlocal* operators nor performing matrix inversions. Our presentation continues in § 4 with a number of demonstrative results that show that our SOR scheme remains equally robust even under extreme non-LTE conditions in very fine grids, often leading to an order of magnitude of saving in the total computational time with respect to the local operator technique. Section 4.4 demonstrates that our G-S method has excellent smoothing capabilities and establishes it as the basic iterative scheme of choice to perform the required smoothing iterations in multigrid RT. Finally, § 5 provides some concluding remarks.

2. BASIC ITERATIVE METHODS

Consider the linear system of algebraic equations

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{b}\,, \tag{1}$$

where $\boldsymbol{A}$ is an operator, $\boldsymbol{b}$ is a known vector, and $\boldsymbol{u}$ is the unknown (e.g., the source function at each grid point). Assume that we have an approximate solution $\boldsymbol{u}^{\rm old}$. Since $\boldsymbol{u}^{\rm old}$ is not the exact solution $\boldsymbol{u}$, we have a nonzero *residual* given by

$$\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{u}^{\rm old} = \boldsymbol{A}\boldsymbol{e}\,, \tag{2}$$

where $\boldsymbol{e} = \boldsymbol{u} - \boldsymbol{u}^{\rm old}$ is the *error* associated with the estimate $\boldsymbol{u}^{\rm old}$. Therefore, one way to find the exact solution $\boldsymbol{u}$ is to obtain the error $\boldsymbol{e}$ by solving the system (2) and then

$$\boldsymbol{u} = \boldsymbol{u}^{\rm old} + \boldsymbol{e}\,. \tag{3}$$

However, to solve the system $\boldsymbol{A}\boldsymbol{e} = \boldsymbol{r}$ is as difficult as solving the original system (1), and nothing would be gained.

A better idea is to obtain an approximate correction e^* by solving

$$A^*e^* = r\,, \tag{4}$$

where A^* is an approximation to the operator A such that this new system is easier to solve than the original one, and then to iterate until convergence is reached. The resulting iterative scheme reads

$$A^*u^{\rm new} = (A^* - A)u^{\rm old} + b\,, \tag{5}$$

or

$$u^{\rm new} = Gu^{\rm old} + w\,, \tag{6}$$

where

$$G = 1 - (A^*)^{-1}A\,, \tag{7}$$

with 1 the identity operator, and the vector

$$w = (A^*)^{-1}b\,. \tag{8}$$

The convergence properties of the scheme depend on the *spectral radius* of the iteration operator G. The spectral radius, ρ, is the largest absolute eigenvalue of G, and it gives the *asymptotic rate of convergence* of the iterative method. In fact, errors decrease as $\rho^{\rm itr}$ (with itr being the iteration number) and, as shown below in equation (30), the number of iterations required to reduce the error by a given factor is inversely proportional to $-\ln(\rho)$. This is because the error e satisfies $e^{\rm new} = Ge^{\rm old}$; therefore, for the method to converge, ρ must be smaller than unity (e.g., Young 1971). Alternatively, one may express the iterative scheme in terms of the corrections Δu as follows:

$$u^{\rm new} = u^{\rm old} + \Delta u\,, \tag{9}$$

where

$$\Delta u = (A^*)^{-1}r\,. \tag{10}$$

It is useful at this stage to choose a particular *reference* problem in order to clarify how these methods can be developed in a way suitable for numerical RT. To this end, we select the coherent scattering case, but note that, as demonstrated by the results presented in § 4.3, the formulae that follow can indeed be generalized and applied straightforwardly to the two-level atom line transfer case for which the relevant quantity is the average profile intensity $\bar{J}$ instead of just the mean intensity J. For the coherent scattering problem the source function vector S is given by (e.g., Mihalas 1978)

$$S = (1 - \epsilon)J + \epsilon B\,, \tag{11}$$

where ϵ is the non-LTE parameter that we assume constant *only* for notational simplicity, and B is the Planck function vector. The mean intensity J can be written as

$$J = \Lambda[S] + \mathcal{J}\,, \tag{12}$$

where the vector $\mathcal{J}$ represents the transmitted contribution to J due to the *given* incident radiation at the boundaries of the computational domain, and Λ is the angle-averaged Λ-operator. Accordingly, the unknown vector u in equation (1) is the source function S, while the right-hand side vector b and the operator A are given by

$$b = \epsilon B + (1 - \epsilon)\mathcal{J}\,, \tag{13}$$

$$A = [1 - (1 - \epsilon)\Lambda]\,. \tag{14}$$

From equation (9), it is now straightforward to show that

$$S^{\rm new} = S^{\rm old} + \Delta S\,, \tag{15}$$

with

$$\Delta S = [1 - (1 - \epsilon)\Lambda^*]^{-1}[(1 - \epsilon)J^{\rm old} + \epsilon B - S^{\rm old}]\,, \tag{16}$$

where Λ^* is the angle-averaged *approximate* Λ-operator and $J^{\rm old} = \Lambda[S^{\rm old}] + \mathcal{J}$.

It is important to clarify the actual meaning of this last expression. The mean intensity vector $J^{\rm old}$ that appears in equation (16) is to be obtained directly via a formal solution of the transfer equation for the given "old" source function values $S^{\rm old}$, i.e., the operator Λ *never* need be evaluated as a matrix itself. Therefore, for *linear* RT problems the strategy currently in use is such that once the *approximate* operator $A^* = 1 - (1 - \epsilon)\Lambda^*$ has been computed and inverted, each iteration just requires a call to a formal solution routine that calculates the mean intensity J_i at each spatial grid point i (see, e.g., Rybicki 1991).

For our discussion below, we establish now the properties of the operator A. From equation (14) it is clear that these properties depend on those of Λ. The physical meaning of this Λ-operator can easily be deduced from equation (12). Considering a discrete spatial grid with the incident intensities at the boundaries of the medium equal to zero, each element Λ_{ij} would be a positive real number between 0 and 1, since it just gives the response of the mean intensity J at the spatial point i due to a unit-pulse source-function perturbation at j. From the formal solution of the transfer equation (see eq. [34] below) it is clear that the elements Λ_{ij} only depend on the optical distances between i and j. For RT problems similar to those considered in this paper (i.e., for plane-parallel semi-infinite atmospheres where the spatial grid index is taken to be unity at the surface and increasing inward), one would find $\Lambda_{ij} > \Lambda_{ji}$ for $j > i$, i.e., the elements of the operator Λ would be more significant in its upper triangular side than in the lower one. Accordingly, considering equation (14), the following may be concluded:

1. The elements of the operator A are real numbers.
2. The operator A is an L-operator, i.e., its diagonal elements $a_{ii} > 0$, and its nondiagonal elements $a_{ij} < 0$.
3. The operator A has *weak diagonal dominance*, i.e., in at least one row the diagonal element is *larger* in absolute value than the absolute sum of the off-diagonal elements, while in the remaining rows the diagonal element is *larger* or *equal* in absolute value than the absolute sum of the off-diagonal elements.

Clearly, the various possible iterative methods result from the selection of the splitting operator A^* (see eqs. [9] and [10]). We point out that properties (1) and (3) suffice to guarantee the convergence of all the iterative schemes we are about to consider (see, e.g., Varga 1962; Young 1971).

2.1. *Picard's or* Λ *Iteration*

This is obtained when the splitting operator A^* in equation (10) is taken equal to the identity operator, implying that Λ^* in equation (16) is to be chosen equal to zero. This means that at each spatial grid point i, the iterative corrections are as simply as follows:

$$S_i^{\rm new} = S_i^{\rm old} + \Delta S_i = S_i^{\rm old} + [(1 - \epsilon)J_i^{\rm old} + \epsilon B_i - S_i^{\rm old}]\,. \tag{17}$$

Therefore, no matrix inversions are required, and the computing time per iteration is the smallest that can be achieved. However, the spectral radius of the iteration operator $\boldsymbol{G} = \mathbf{1} - \boldsymbol{A} = (1 - \epsilon)\boldsymbol{\Lambda}$ (see eqs. [7] and [14]) is $\rho(\boldsymbol{G}) \approx 1 - \epsilon$ for optically thick media; therefore, as it can also be understood from physical arguments (see, e.g., Mihalas 1978), the method converges extremely slowly for non-LTE problems of practical interest, since for these cases $\rho(\boldsymbol{G}) \approx 1$.

2.2. *Jacobi's Method*

This iterative scheme (Jacobi 1845) is obtained when the splitting operator $\boldsymbol{A}^*$ is given by the exact diagonal of the true operator $\boldsymbol{A}$, and hence $\boldsymbol{\Lambda}^*$ in equation (16) must be chosen equal to the diagonal of $\boldsymbol{\Lambda}$. Since the splitting operator $\boldsymbol{A}^*$ is *local* (i.e., diagonal), its inverse is just the scalar inverse of its elements, and the computing time per iteration is also the smallest that can be achieved. The diagonal of the true operator $\boldsymbol{A}$ actually constitutes the optimal *local* operator available, and accordingly convergence properties are substantially better than those in Picard's scheme. In fact, in an important paper OAB (1986) demonstrated that Jacobi's iterative scheme can be used as a practical method for solving RT problems, specially if it is combined with powerful acceleration of convergence techniques, such as those discussed by Auer (1987, 1991).

As can be deduced from equations (9) and (10), the Jacobi iteration uses $\boldsymbol{u}^{\rm old}$ to compute $u_1^{\rm new}, u_2^{\rm new}, \ldots u_N^{\rm new}$ (with N being the number of spatial grid points) as follows (the reason for splitting the summation as we do here will become evident below):

$$u_i^{\rm new} = u_i^{\rm old} + \frac{b_i - \sum_{j=1}^{i-1} a_{ij} u_j^{\rm old} - \sum_{j=i}^{N} a_{ij} u_j^{\rm old}}{a_{ii}}, \qquad (18)$$

where a_{ij} are the elements of the operator $\boldsymbol{A}$. For our RT reference problem we have, *at each spatial point*:

$$S_i^{\rm new} = S_i^{\rm old} + \Delta S_i, \qquad (19)$$

with

$$\Delta S_i = \frac{[(1 - \epsilon) J_i^{\rm old} + \epsilon B_i - S_i^{\rm old}]}{[1 - (1 - \epsilon)\Lambda_{ii}]}. \qquad (20)$$

Therefore, as with the Λ-iteration, each Jacobi iteration simply requires a single formal solution of the transfer equation for the previous estimate $\boldsymbol{S}^{\rm old}$ of the source function, in order to provide the mean intensity $\boldsymbol{J}^{\rm old}$. Note that the approximate operator here (i.e., the diagonal elements Λ_{ii} of the full operator $\boldsymbol{\Lambda}$) can be obtained efficiently. For example, if the formal solution technique proposed by Kunasz & Auer (1988) is selected, a suitable strategy for obtaining Λ_{ii} is available (Olson & Kunasz 1987; Auer & Paletou 1994), while the reader is referred to the appendix of Rybicki & Hummer's (1991) paper if Feautrier's method is chosen.

2.3. *Gauss-Seidel Method*

The (G-S) method (Seidel 1874) is obtained when $u_j^{\rm old}$ is replaced by $u_j^{\rm new}$ in the first sum of equation (18). The resulting iterative scheme reads

$$u_i^{\rm new} = u_i^{\rm old} + \frac{b_i - \sum_{j=1}^{i-1} a_{ij} u_j^{\rm new} - \sum_{j=i}^{N} a_{ij} u_j^{\rm old}}{a_{ii}}. \qquad (21)$$

This equation can easily be reorganized to express it in the following way:

$$\sum_{j=1}^{i} a_{ij} u_j^{\rm new} = b_i - \sum_{j=i+1}^{N} a_{ij} u_j^{\rm old}, \qquad (22)$$

which shows directly (see eq. [5]) that the ensuing approximate operator $\boldsymbol{A}^*$ is given by the *lower* triangular part of the true operator $\boldsymbol{A}$, i.e., it is formed by the elements that are on the diagonal and beneath the diagonal of the full operator $\boldsymbol{A}$. Note that the same applies here to $\boldsymbol{\Lambda}^*$ with respect to $\boldsymbol{\Lambda}$, because $\boldsymbol{A}$ is given by equation (14). Therefore, a small change in the Jacobi iterative scheme has produced a crucial change in the approximate operator $\boldsymbol{\Lambda}^*$, which is now *nonlocal*, and it represents a much better approximation to the true operator $\boldsymbol{\Lambda}$.

For our RT reference problem the G-S source function corrections at each spatial grid point i would be

$$\Delta S_i^{GS} = \frac{[(1 - \epsilon) J_i^{\rm old\ and\ new} + \epsilon B_i - S_i^{\rm old}]}{[1 - (1 - \epsilon)\Lambda_{ii}]}, \qquad (23)$$

where $J_i^{\rm old\ and\ new}$ means that at the spatial point i the mean intensity has to be calculated via a formal solution of the transfer equation using the "new" source function values $S_j^{\rm new}$ already obtained at points $j = 1, 2, \ldots, i - 1$, and the "old" source function values $S_j^{\rm old}$ at points $j = i, i + 1, \ldots, N$. It is very important to clarify the meaning of equation (23):

1. First, at point $i = 1$ (which can freely be assigned to any of the two boundaries of the medium under consideration) use "old" source function values to calculate J_1 via a formal solution. Apply equation (23) to calculate $S_1^{\rm new}$.
2. Go to the next point $i = 2$ and use $S_1^{\rm new}$ and the "old" source-function values $S_j^{\rm old}$ at points $j = 2, 3, \ldots, N$ to get J_2 via a formal solution. Apply equation (23) to calculate $S_2^{\rm new}$.
3. Go to the next spatial point k and use the previously obtained "new" source function values at $j = 1, 2, \ldots, k - 1$, but still the "old" ones at $j = k, k + 1, \ldots, N$ to get J_k via a formal solution and $S_k^{\rm new}$ as dictated by equation (23).
4. Go to the next point $k + 1$ and repeat what has just been indicated in the previous point until arriving to the other boundary point.

The result of doing what we have just summarized is a G-S iteration, i.e., it gives exactly the next value for $S^{\rm new}$ that equations (15) and (16) would provide directly, were the approximate operator $\boldsymbol{\Lambda}^*$ chosen equal to the lower (or upper!) triangular part of $\boldsymbol{\Lambda}$. (Note that it would be the *lower* triangular part of $\boldsymbol{\Lambda}$ if, for a *fixed* numbering of the grid points, we start the above-mentioned process at $i = 1$, while it would be the *upper* triangular part if we started at $i = N$.) It is very important to emphasize that, although the convergence rate of the resulting scheme actually corresponds to the above-mentioned *nonlocal* triangular operator, performing our G-S iterations (see eq. [23]) neither requires the construction of such a nonlocal operator nor the application of any matrix inversion procedure. The difference with respect to Jacobi's iteration is that in that case, given $\boldsymbol{S}^{\rm old}$, one first performs a formal solution of the transfer equation to obtain $\boldsymbol{J}^{\rm old}$ and then applies equation (20) for the source function corrections, while with our G-S scheme (see eq. [23]) each time a "new" source function value $S_i^{\rm new}$ is obtained at a point i, one uses it when calculating the mean intensity J_{i+1} at the next grid point $i + 1$, which is required to get $S_{i+1}^{\rm new}$, and so on. Clearly, the only way to do this *efficiently* is via the development of a suitable strategy that

allows to carry out G-S iterations (see eq. [23]) (i.e., to do what we have summarized in the four points above) in the same amount of computing time as that required by each Jacobi iteration. This will be the objective of the next section.

2.4. *The Successive Overrelaxation Method*

The SOR method (Young 1950, 1971) is obtained from the G-S iteration (21) via the use of a parameter ω (with $1 < \omega < 2$) as follows:

$$u_i^{\rm new} = u_i^{\rm old} + \omega\left(\frac{b_i - \sum_{j=1}^{i-1} a_{ij} u_j^{\rm new} - \sum_{j=i}^{N} a_{ij} u_j^{\rm old}}{a_{ii}}\right). \quad (24)$$

Accordingly, for our RT example the SOR correction at each spatial point i would be

$$\Delta S_i^{\rm SOR} = \omega \, \Delta S_i^{\rm GS}, \quad (25)$$

which shows that SOR's method *overcorrects* the value of S at the current stage of the G-S iteration, thus anticipating future corrections. It is straightforward to show that the ensuing splitting operator $\boldsymbol{A}^*$ is just the G-S $\boldsymbol{A}^*$, which, as explained above, is the lower (or upper) triangular part of $\boldsymbol{A}$, but now its diagonal elements are divided by ω. However, it is important to note from equation (14) that this *does not* imply that the diagonal elements of the ensuing approximate operator $\boldsymbol{\Lambda}^*$ are simply Λ_{ii}/ω.

The best choice for the relaxation parameter ω is that which leads to the highest rate of convergence, i.e., that which minimizes the largest absolute eigenvalue of the operator $\boldsymbol{G}$ (see eq. [7]). There is a very important theorem (Young 1971) that establishes that, if the operator $\boldsymbol{A}$ is "consistently ordered" (see Hageman & Young 1981), the optimal value of ω is given by

$$\omega_{\rm opt} = \frac{2}{1 + \sqrt{1 - \delta}}, \quad (26)$$

where δ is the spectral radius of the G-S iteration. In general, from a strict point of view, the operator $\boldsymbol{A}$ (see eq. [14]) encountered when solving RT problems is not consistently ordered. However, equation (26) is still valid if Jacobi's method converges and its corresponding iteration operator $\boldsymbol{G}$ has real eigenvalues (see, e.g., Young & Gregory 1972). Moreover, as shown by Kahan (1958), if $\boldsymbol{A}$ is an L-operator (cf. property b above) and if one uses the ω-value resulting from equation (26), then the largest absolute eigenvalue α of the iteration operator $\boldsymbol{G}$ (see eq. [7]) of the SOR method is such that

$$\omega_{\rm opt} - 1 \le \alpha \le \sqrt{\omega_{\rm opt} - 1}, \quad (27)$$

with the equality

$$\alpha = \omega_{\rm opt} - 1 = \frac{1 - \sqrt{1 - \delta}}{1 + \sqrt{1 - \delta}} \quad (28)$$

possible *only* if all eigenvalues of $\boldsymbol{G}$ have modulus $|\omega_{\rm opt} - 1|$. With the demonstrative results of § 4 we shall confirm that equations (26) and (27) are indeed effective in numerical RT. Our purpose now is to demonstrate that with a RT method based on these optimal SOR iterations one can obtain an order-of-magnitude improvement over the Jacobi-based optimal local operator method.

To this end, we note that in order to reduce the error by a factor 10^{-f} using an iterative method of spectral radius ρ, we have to iterate $N_{\rm iter}$ times, which we obtain from

$$\rho^{N_{\rm iter}} = 10^{-f}, \quad (29)$$

which in turn leads to

$$N_{\rm iter} = -\frac{f \ln(10)}{\ln(\rho)}. \quad (30)$$

As shown below, for RT problems the variation of the spectral radius λ of Jacobi's method with the number n of grid points per decade in optical depth can be well approximated by

$$\lambda = 1 - \frac{a}{n^b}, \quad (31)$$

where a and b are constants whose particular values depend on ϵ, but are of order unity. Therefore, according to equation (30) the number of Jacobi iterations required to reduce the error by a given factor is (for $n \gg 1$) as follows:

$$N_{\rm iter}({\rm Jacobi}) \approx \frac{f}{a} \ln(10) n^b, \quad (32)$$

while, taking into account equations (27) and (28), and that $\delta \approx \lambda^2$, the number of necessary SOR iterations is only

$$\frac{1}{2}\frac{f}{\sqrt{2a}} \ln(10) \sqrt{n^b} \le N_{\rm iter}({\rm SOR}) \le \frac{f}{\sqrt{2a}} \ln(10) \sqrt{n^b}. \quad (33)$$

This result leads to the conclusion that an impressive amount of CPU time can be saved if one is able to develop a suitable strategy for performing SOR iterations at the same amount of computational cost as that required by Jacobi's method (see next section). Further, note that the pure G-S scheme already yields a factor of 2 saving with respect to Jacobi's method because $\delta \approx \lambda^2$.

As may be expected, the effectiveness of the SOR method depends on the availability of a prescription for selecting the *optimal* parameter ω. Fortunately, as already mentioned (see the demonstrative results below), equation (26) is effective for RT problems. Therefore, it is only necessary to establish a suitable procedure for estimating δ from which to derive the value of ω. We shall indicate a simple procedure for doing this, which will allow us to demonstrate that our SOR method is competitive with the best acceleration methods applied to Jacobi's scheme.

3. EFFICIENT IMPLEMENTATION OF THE GAUSS-SEIDEL AND SUCCESSIVE OVERRELAXATION METHODS

The objective here is to describe the method that we have developed for performing G-S and SOR iterations at the same computational cost required by Jacobi's method. (By "computational cost required by each Jacobi iteration" we mean that which can be achieved when both the diagonal elements Λ_{ii} and the mean intensities J_i are calculated within the framework of the formal solution strategy selected). In our presentation we need only to refer to G-S iterations since the SOR corrections are straightforwardly obtained from the G-S ones as indicated by equation (25). A G-S iteration is achieved once the source function corrections (see eq. [23]) are obtained at all grid points. This, in turn, requires implementing the procedure summarized in § 2.3 in order to calculate the mean intensities $J_i^{\rm old\ and\ new}$ at all grid points i. Clearly, we need to develop a formal solution routine such that each call to it produces as an output a truly G-S iteration. To this end, one has to carry out the source function corrections (see eqs. [19] and [23]) within the formal solution solver itself so that, once $S_i^{\rm new}$ is obtained at the grid point i being considered, the mean

intensity J_{i+1} at the following point $i+1$ can be calculated using these "new" source function values from the grid points considered *previously*, but still using the "old" source function values of the remaining points.

Consider an arbitrary distribution of spatial grid points, like the one depicted in Figure 1. Points 1 and N are the two boundary grid points, at which the specific intensities $I(\mu)$ for rays *entering* the medium are given ($\mu = \cos\theta$, with θ being the angle the ray makes with the normal to the surface); for instance, for the plane-parallel atmosphere examples considered in this paper, point 1 would be the surface point where the incoming intensity is 0, while point N would be the lower boundary point where the specific intensity is given by the diffusion approximation. Choosing the so-called short-characteristics integration technique (see Kunasz & Auer 1988) as a formal solution strategy of the RT equation, the specific intensity at a given point O, for a given frequency and ray direction, can be expressed as

$$I_O = I_M e^{-\Delta\tau_M} + \Psi_M S_M + \Psi_O S_O + \Psi_P S_P , \qquad (34)$$

where $\Delta\tau_M$ is the optical distance on segment MO, and the Ψ-quantities are functions of the optical distances between O and the *upwind* point M and between O and the *downwind* point P, while S_k (with $k = M$, O, or P) are the source function values at such grid points k. Formula (34) assumes that the source function varies *parabolically* along the points M, O, and P. Alternatively, one may be tempted to assume that the source-function varies *linearly* along M and O, in which case the last term of equation (34) would disappear, and the quantities Ψ_M and Ψ_O would only depend on $\Delta\tau_M$. Our development below is for the truly accurate *parabolic* case, in which formula (34) is applied to obtain the radiation intensity at the *interior* grid points, while the above-mentioned *linear* formula is *only* used at the boundary grid points for rays going out of these boundaries.

To facilitate the understanding of our G-S method, it is convenient to describe it in two distinct parts: an *incoming* one and an *outgoing* one, which are separated by a *lower boundary* section.

1. *Incoming part.*—After taking into account the upper boundary contribution, the calculation starts at point 2, progressing point by point until the lower boundary one. At each of these spatial points k the *incoming* intensity $I(\mu)$ is calculated according to equation (34) for each *incoming* angle $\mu < 0$ of the angular quadrature chosen for the numerical solution of the problem. These intensities are actually used at each grid point k in order to make an *incoming* contribution to the mean intensity. Therefore, at the end of the *incoming* section, the content of the mean intensity array J_k is

$$J_k = J_k^{\rm in} = \tfrac{1}{2}\int_{-1}^{0} I(\mu)\,d\mu , \qquad (35)$$

where k is the spatial grid-point index. As explained below, with the exception of the two boundary points, for the moment the array J_k only contains an *approximation* to the exact *incoming* contribution to the mean intensity at the current iterative stage.

2. *Lower boundary section.*—At the lower boundary point ($k = N$), the content of the array J_N is the exact $J_N^{\rm in}$. At this point ($k = N$) the *outgoing* intensities are determined already

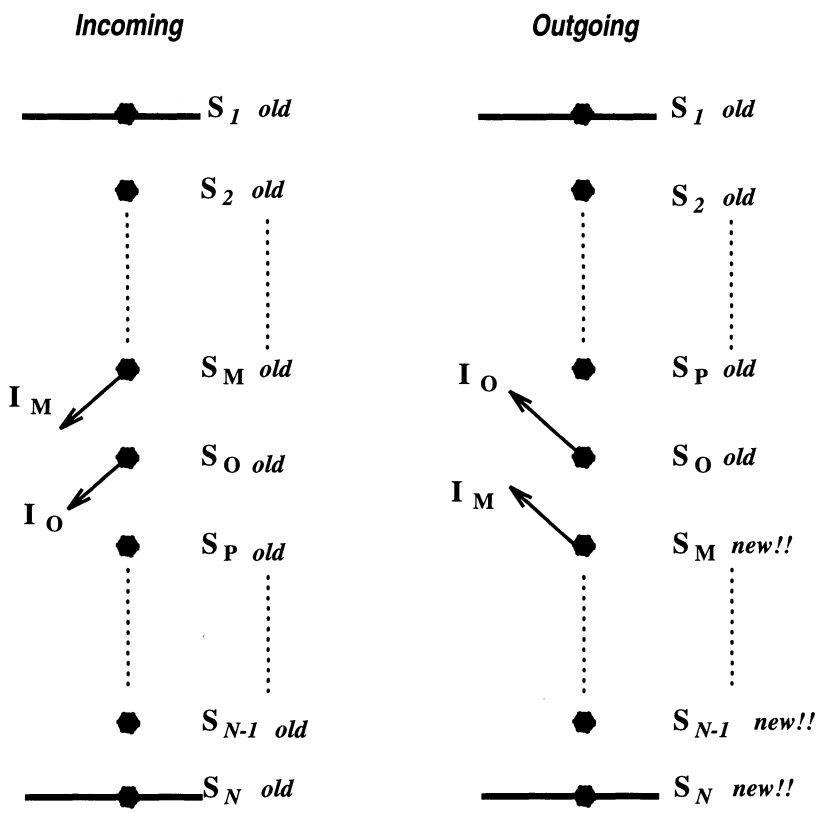

FIG. 1.—One-dimensional spatial grid with short characteristics M–O providing a schematic visualization of the *incoming* part (1) and the *outgoing* part (3) of the G-S strategy described in the text.

by the lower boundary condition. Therefore, it is straightforward to use this information to calculate the *outgoing* contribution to the mean intensity, i.e.,

$$J_N^{\rm out} = \tfrac{1}{2}\int_0^1 I(\mu)d\mu\ . \tag{36}$$

Given the mean intensity $J_N = J_N^{\rm in} + J_N^{\rm out}$, we can find (via eqs. [19], [23], or [25]) the source function correction ΔS_N and the "new" source function value $S_N^{\rm new}$ at point $k = N$. Note that this $J_N = J_N^{\rm old}$, since for the point where the first correction is made only "old" source function values are available.

3. *Outgoing part.*—This starts at grid point $N-1$ and advances point by point, calculating the G-S source function corrections (see eq. [23]) until it reaches the upper boundary. To this end, the *outgoing* intensity at point $O = N-1$, for each *outgoing* angle ($\uparrow$), is first calculated according to equation (34), but noting that here the upwind point (M) is now N, and the downwind point (P) is $N-2$. Note that the source function value at M is the $S_N^{\rm new}$ that has just been obtained in the preceding step, while $S_O = S_{N-1}^{\rm old}$ and $S_P = S_{N-2}^{\rm old}$. Therefore,

$$I_{N-1}(\uparrow) = I_N(\uparrow)e^{-\Delta\tau_N(\uparrow)} + \Psi_N(\uparrow)S_N^{\rm new} + \Psi_{N-1}(\uparrow)S_{N-1}^{\rm old} + \Psi_{N-2}(\uparrow)S_{N-2}^{\rm old}\ . \tag{37}$$

After taking into account the contributions for all the *outgoing* angles ($\uparrow$), it would be possible to obtain, as in equation (36), the *outgoing* mean-intensity contribution $J_{N-1}^{\rm out}$. However, in order to obtain the correct *total* mean intensity $J_{N-1}^{\rm old\ and\ new}$, one has to remember, from the *incoming* section, that the J_k array only contains *part* of the true *incoming* contribution to the mean intensity. In fact, what was stored in array J_k in the *incoming* section was only an *approximation* to the correct *incoming* mean-intensity contribution, simply because $I_{N-1}(\downarrow)$ was calculated there as follows:

$$I_{N-1}(\downarrow) = I_{N-2}(\downarrow)e^{-\Delta\tau_{N-2}(\downarrow)} + \Psi_{N-2}(\downarrow)S_{N-2}^{\rm old} + \Psi_{N-1}(\downarrow)S_{N-1}^{\rm old} + \Psi_N(\downarrow)S_N^{\rm OLD}\ , \tag{38}$$

i.e., using $S_N^{\rm OLD}$ instead of what is actually required, namely, the "new" $S_N^{\rm new}$ value obtained in the lower boundary section. Therefore, all we have to do in the present *outgoing* section in order to end up with the correct mean intensity $J_{N-1}^{\rm old\ and\ new}$ into array J_k (for the moment at $k = N-1$) is to add the following contribution to the J_k array:

$$J_k^{\rm out} + \Delta J_k^{\rm in} = \tfrac{1}{2}\left[\int_0^1 I(\mu)d\mu + \Delta S_{k+1}\int_{-1}^0 \Psi_{k+1}(\downarrow)d\mu\right], \tag{39}$$

which can actually be done rapidly because the correction ΔS_{k+1} and the quantities $\Psi_P = \Psi_{k+1}(\downarrow)$ are available from previous computational steps. (Note, however, that the contributions $\Delta J_k^{\rm in}$ of eq. [39] would be 0 if instead of the *parabolic* formal solution formula [34] the *linear* one—i.e., equation [34] with $\Psi_P = 0$—were used). Having obtained $J_k^{\rm old\ and\ new}$ (at $k = N-1$), it is straightforward to apply equations (23) and (19) to obtain the correction ΔS_{N-1} and the source function $S_{N-1}^{\rm new}$.

Before passing to the next point $O = k-1$ (e.g., to $O = N-2$ if the previous point $k = N-1$) for calculating its corresponding "new" source function value via the repetition of the very same steps that we have just described, it is imperative to *add* (for each *outgoing* angle) the following correction term to the specific intensity array $I_k^{\rm out}(\mu)$:

$$\Delta I_k^{\rm out}(\mu) = \Psi_k(\uparrow)\Delta S_k\ , \tag{40}$$

where both $\Delta S_k = S_k^{\rm new} - S_k^{\rm old}$ and $\Psi_k(\uparrow)$ are available from previous computational steps. These intensities $I_k^{\rm out}(\mu)$ play the role of the *upwind* intensities I_M, which appear in equation (34) once we apply this very equation to obtain the specific intensities at such next point $O = k-1$. Clearly, we have to make these specific intensity corrections before going to each next point in order to take into account that the "new" source function $S_k^{\rm new}$ has just been obtained at the previous point k. Updating the upwind *outgoing* specific intensities according to equation (40) is very important. If waived, the resulting scheme would converge at a significantly slower rate, and the ensuing iterations would not be truly G-S iterations.

In this efficient way one moves point by point upward doing the source function corrections as dictated by equations (23) or (25), so that each call to our formal solution routine produces a G-S or SOR iteration after a computing time similar to that required by Jacobi iterations.

For the line transfer case the relevant quantity is the average profile intensity $\bar{J} = \frac{1}{2}\int_{-1}^1 d\mu \int d\nu\phi(\nu,\mu)I(\nu,\mu)$ [with the absorption profile $\phi(\nu,\mu)$], but the whole process remains unaltered, with the exception of having to consider not only each ray direction, but also the profile-weighted contribution at each frequency ν.

4. DEMONSTRATIVE RESULTS

This section is aimed at demonstrating the performance and convergence properties of our G-S and SOR RT methods in comparison with those of the broadly used Jacobi-based OAB technique. To this end, we choose as benchmark problems the coherent scattering and the two-level atom complete redistribution cases for the constant property atmosphere limit, noting that similar results have been obtained for more general situations.

4.1. *The Coherent Scattering Problem*

The coherent scattering source function is given by equation (11), where $\boldsymbol{J}$ is the mean intensity, $\boldsymbol{B}$ is the Planck function (which we assume equal to unity) and ϵ is the non-LTE parameter, which we assume constant. Figure 2 shows the final result of the iterative solution performed with any of the three methods (i.e., Jacobi, G-S, and SOR) for various values of ϵ.

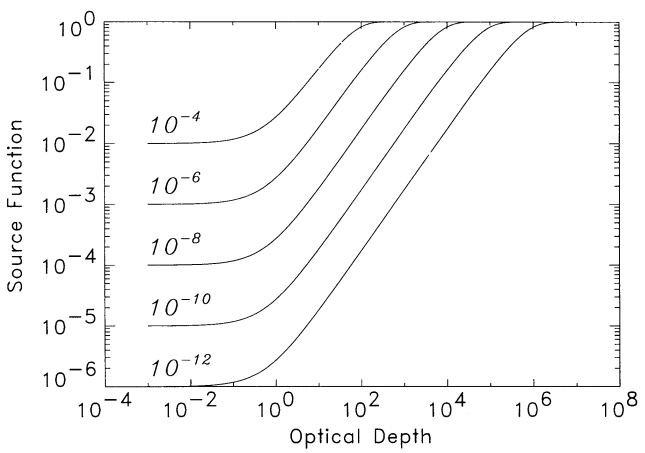

FIG. 2.—The run of the source function with optical depth for the coherent-scattering isothermal-atmosphere problem with the indicated values of ϵ. The three solution methods used (i.e., the Jacobi-based OAB-technique and our G-S and SOR methods) give the same solution, which agrees with the analytical result.

The calculations were carried out using a one-point angular quadrature with $\mu = \pm 1/\sqrt{3}$, which is equivalent to Eddington's approximation. In this way we can compare directly the numerical results for the run of the source function with optical depth with the *analytical* result also overplotted in Figure 2. This analytical solution can easily be obtained if one invokes Eddington's approximation (see Mihalas 1978, p. 149).

The excellent agreement in Figure 2 between the analytical and any of the three numerical results indicates that the operator splitting methods considered in § 2 are all capable, in principle, of providing the correct answer, even for very small values of the non-LTE parameter ϵ. However, it says nothing about the efficiency and convergence properties of the methods themselves. For that purpose we show the variation with the iteration number (itr) of the relative *true error* T_e, which we define by

$$T_e(n, \text{itr}) = \max \left| \frac{S(n, \text{itr}) - S}{S} \right| . \quad (41)$$

Here, the source function S denotes the above-mentioned analytical result, and n indicates the number of grid points per decade in optical depth. At the iterative stage "itr", T_e gives the *maximum* absolute relative error among all the source-function values corresponding to each of the spatial grid points. It is clear that as one iterates using a convergent method, the true error T_e decreases until the *truncation error* of the grid being used is reached. At this iterative stage the T_e versus itr curve becomes horizontal and no further decrease takes place, simply because each grid of a given resolution level has associated with it a *truncation error* [denoted by $T_e(n, \infty)$], which is equal to the accuracy that the chosen grid and formal solution method can provide. This is shown in Figure 3 for the case with $\epsilon = 10^{-6}$ and for a grid with nine points per decade. With the exception of the curve corresponding to the poorly convergent Λ-iteration procedure, the remaining curves (i.e., the ones for Jacobi, G-S, and SOR) become horizontal at $T_e \approx 3.5 \times 10^{-3}$, which tells us that the accuracy of the solution in the chosen grid is well below 1% when the parabolic short-characteristics formal solution formula is adopted (see eq. [34]). For the comparative purposes that follow, we use the criterion that the number of iterations required to reach convergence is given by the number of iterations at which the true error curve becomes horizontal. In this respect, an accurate and practical criterion for deciding when the iterative process should be terminated has been presented by Auer et al. (1994).

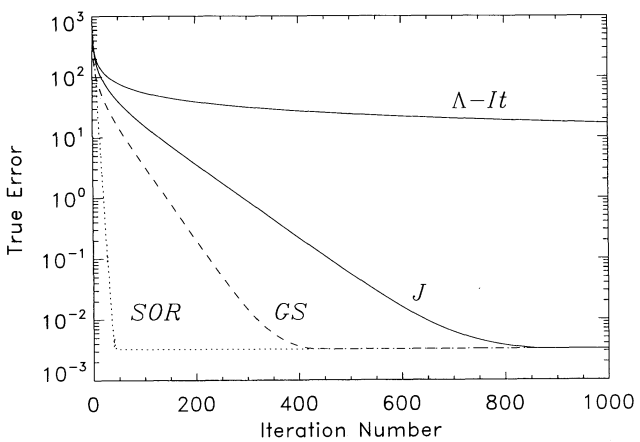

FIG. 3.—Typical convergence properties of the various iterative schemes considered are demonstrated in this coherent scattering example, where $\epsilon = 10^{-6}$ and the chosen grid has $n = 9$ points per decade.

As expected from the previous discussion in § 2.4, the number of iterations that have to be performed to reach convergence by means of the G-S method is a factor 2 smaller than with Jacobi's, while the number of iterations required by our SOR method is about a factor 20 smaller (see Fig. 3). It is very important to emphasize that this saving in terms of the number of required iterations implies exactly the same saving regarding the total CPU time, since the procedure described in the previous section actually allows G-S and SOR iterations to be carried out virtually at the same computational cost as that required by Jacobi's method. This very important saving agrees with that predicted by our order-of-magnitude estimates (see eqs. [32] and [33]). To check this, Figure 4 shows the variation of the largest absolute eigenvalue (λ) of Jacobi's method (obtained as explained below) with the number n of points per decade. The solid lines in Figure 4 are the fits to λ, obtained according to equation (31) for the values of a and b indicated. In this figure we also include the variation of δ and α, which are, respectively, the largest absolute eigenvalues of our G-S and SOR methods.

It is important to emphasize that the spectral radius ρ provides a measure of the *asymptotic convergence rate* (see eq. [30]). The values of ρ (either λ for Jacobi, δ for pure G-S or α for the SOR method) shown in Figure 4 are actually the estimates of the spectral radius for the corresponding iteration operator $\boldsymbol{G}$ (see eq. [7]) obtained after calculating, for itr $\gg 1$, the ratio $R_c(\text{itr} + 1)/R_c(\text{itr})$, where R_c is the maximum relative *change*. This actually leads to a reasonably good estimate of ρ since, from equation (6), the change $\Delta \boldsymbol{u}(\text{itr} + 1) = \boldsymbol{G}\Delta \boldsymbol{u}(\text{itr})$, the iterations converge to the eigenvector corresponding to the dominant eigenvalue, and the magnitude of this eigenvalue is the spectral radius ρ. This, in turn, reveals a practical procedure to estimate the value of ω_{opt} for SOR: after a few pure G-S iterations, one estimates δ as indicated [i.e., $\delta = R_c(\text{itr} + 1)/R_c(\text{itr})$] and then applies equation (26) to obtain the ω-value; finally, one continues iterating doing the corrections as in equation (25). We have carried out a number of test calculations in order to ascertain the number of pure G-S iterations that have to be performed before the application of the above estimation procedure for ω_{opt} can actually yield the truly *optimal* ω-value. We find that, typically, one has to wait until the maximum relative change $\boldsymbol{R}_c$ is well below 0.1; for example, for the fine-grid case shown in Figure 3 this implies about 20 pure G-S iterations. The lower and upper dotted lines in Figure 4 show the lower ($\alpha = \omega_{\text{opt}} - 1$) and upper [$\alpha = (\omega_{\text{opt}} - 1)^{1/2}$] limits for α as established by equation (27). As expected, the estimated α-eigenvalues given by the symbols lie within these two limits, while λ and δ are related according to $\delta \approx \lambda^2$.

It is now of interest to show the sensitivity of our SOR method to the parameter ω. An example is shown in Figure 5 for a grid with 4.5 points per decade and for $\epsilon = 10^{-6}$. The value for ω_{opt} is 1.52 and it is indeed the one that, as shown in Figure 5*a*, leads to the fastest convergence. The convergence rates for other ω-values lie between this optimal rate and that provided by pure G-S iterations. An alternative illustration is shown in Figure 5*b*, where the estimated largest absolute eigenvalue α is given against the parameter ω. We first point out that, in accordance with mathematical theory (e.g., Young & Gregory 1972), a necessary condition for the convergence of

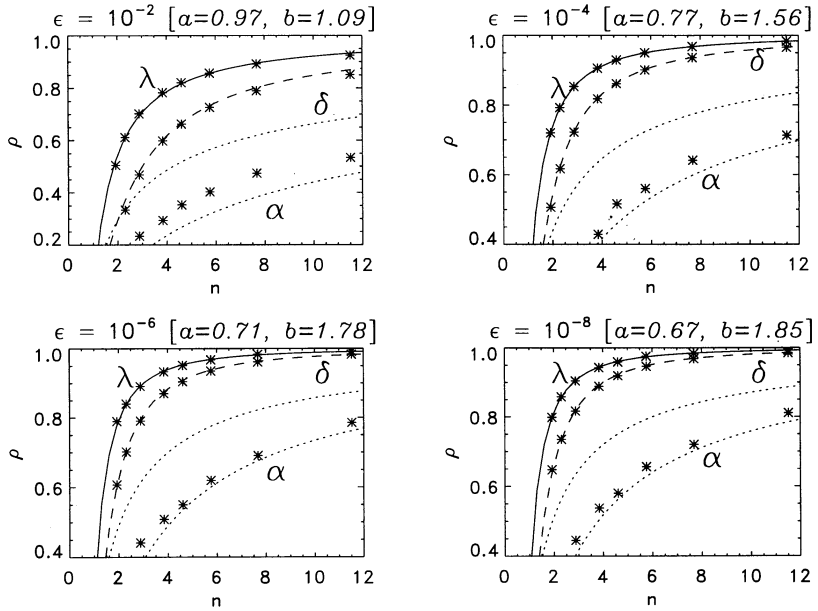

FIG. 4.—The variation of the largest absolute eigenvalues λ (for Jacobi), δ (for G-S), and α (for SOR) with the number n of points per decade for the coherent scattering problem. For each method the symbols give the estimated eigenvalues as described in the text, while the solid line gives the fit to the estimated λ values according to eq. (31) (with the values of a and b indicated). The dashed line is $\delta = \lambda^2$, while, in accordance with eq. (27), the two dotted lines indicate $\alpha = \omega_{opt} - 1$ (the lower limit for α) and $\alpha = (\omega_{opt} - 1)^{1/2}$ (the upper limit for α).

the SOR method is that $0 < \omega < 2$. For $0 < \omega < 1$ we actually have a successive *underrelaxation* RT method. As shown in Figure 5*b*, for $0 < \omega < 1$ the convergence rate is worse than for the G-S $\omega = 1$ case, and faster convergence is only possible for *overrelaxation*, i.e., for $1 < \omega < 2$. The minimum α-value in Figure 5*b* occurs precisely at the ω-value obtained from equation (26), i.e., at $\omega \approx 1.52$. Therefore, although the sensitivity is significant, the selection criterion for the parameter ω is robust enough to guarantee the effectiveness of our SOR method.

4.2. *The Role of Acceleration Techniques*

In order to more than double its speed, the Jacobi-based method of OAB is currently combined with some powerful acceleration of convergence techniques (see Auer 1987, 1991). Therefore, since the SOR method may be considered as a well-founded "extrapolation to the future" of the G-S iterations, it is imperative to compare it with the methods that result from combining the G-S and Jacobi's schemes with such acceleration techniques. This is what we show in Figure 6, again for $\epsilon = 10^{-6}$ and for a very fine grid with nine points per decade. For this example, the figure shows that Ng's acceleration method is effective in improving the convergence rate of both Jacobi's and G-S methods. Notwithstanding, as seen in the figure, the SOR method is still the best, reaching for this example the converged solution at least 4 times quicker than with the method that results from combining Jacobi with Ng.

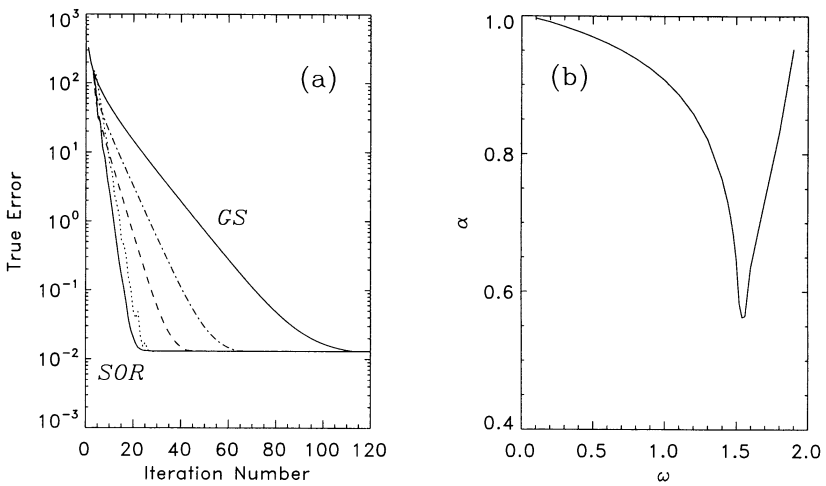

FIG. 5.—The sensitivity of the convergence properties of our SOR method to the parameter ω for the coherent scattering problem with $\epsilon = 10^{-6}$ and $n = 4.5$. The estimated ω-value according to the strategy described in the text is 1.52, which is the optimal one in practice, since it leads to the fastest convergence (see the solid line with the label SOR in [*a*] and note the position of the minimum of the α-curve in [b]). The dotted line corresponds to $\omega = 1.6$, the dashed line to $\omega = 1.4$, and the dash-dotted line to $\omega = 1.25$.

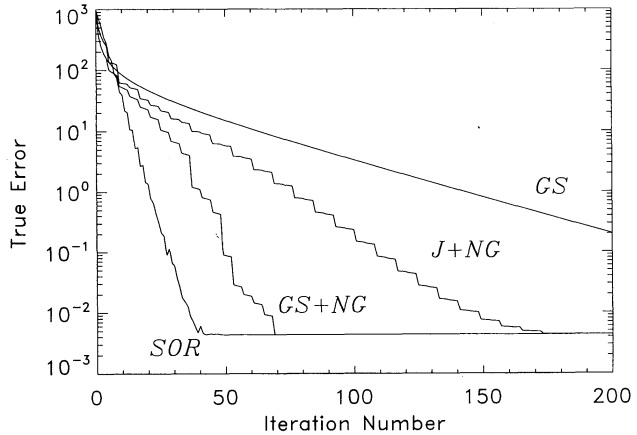

FIG. 6.—The convergence properties of our G-S and SOR methods in comparison with those resulting from combining the Jacobi and G-S schemes with Ng's acceleration of convergence technique. The non-LTE parameter $\epsilon = 10^{-6}$, and $n = 9$.

A similar conclusion is obtained if, instead of Ng, Orthomin's acceleration (Vinsome 1976; Klein et al. 1989; Auer 1991) is used.

It is interesting to point out that when the non-LTE effects are very pronounced (i.e., ϵ very small) and/or the spatial grid used is very fine, as shown in Figure 7, the effectiveness of the acceleration techniques applied to Jacobi's scheme is significantly reduced, but our SOR solution method remains equally robust, implying again gaining factors of about an order of magnitude. Moreover, it is important to remark that, contrary to what happens with our SOR method, the Ng and Orthomin acceleration techniques both require the storage of a number of arrays the size of the system and an extra (although comparatively small) amount of computing time per iteration. Therefore, our SOR method not only leads to much faster convergence, but it also appears to be sufficiently robust to handle complicated non-LTE radiation transfer problems in very fine grids.

On the other hand, the method that results from combining our G-S scheme with such acceleration techniques is very powerful. As can be seen in the last two figures, this often leads to a performance not too far away from that of the SOR method. Further, one must note that in these figures, the

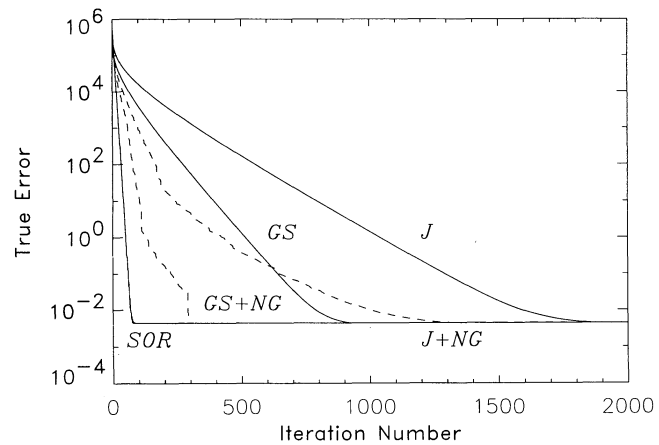

FIG. 7.—Same as in Fig. 6, but for $\epsilon = 10^{-12}$

number of iterations required by SOR to reach convergence is actually the smallest possible one, simply because we have carried out the calculations using the ω_{opt}-value from the very beginning. However, in practical applications the number of required iterations is always somewhat larger. This happens either because one applies SOR from the very beginning by using a nonoptimal ω-value as in Figure 5*a* (e.g., estimating it via eq. [26] using eq. [31] as fitting formula for δ with $a \approx b \approx 1$) or because one carries out a few pure G-S iterations before applying SOR with the optimal ω-value. (The possibility of minimizing this number of pure G-S iterations by using *a priori* estimates of ω and then updating as one converges will be addressed in a future paper.)

4.3. *The Line Transfer Problem*

In Figure 8 we show the variation with the number of points per decade of the largest absolute eigenvalue ρ of Jacobi ($\rho = \lambda$), G-S ($\rho = \delta$), and SOR ($\rho = \alpha$) methods for the standard two-level atom line transfer problem with a Gaussian absorption profile. Compared with the coherent scattering eigenvalues of Figure 4, we note that the ρ values for the line transfer problem are smaller. As can be deduced from Figure 8 the various eigenvalues are related as dictated by $\delta \approx \lambda^2$ and by the limits set by equation (27).

The last point to be noted is that, as discussed in § 3, our G-S and SOR methods can be implemented either starting the source function corrections at the surface or at the lower boundary. As mentioned before, in this latter case the *nonlocal* approximate operator corresponding to the G-S method is the *upper* triangular part of the full Λ-operator, while in the former case Λ^* is the *lower* triangular part of Λ. In Figure 8 we show both δ for the *upper* triangular case (*solid δ-line*) and for the *lower* triangular one (*dashed δ-line*). It is not surprising that, as seen in the figure, starting the corrections at the lower boundary turns out to be slightly more efficient since, as pointed out when discussing the physical meaning of the Λ-operator, the *upper* triangular part of Λ is more significant than the *lower* triangular one. This is, in fact the reason why Scharmer's (1981) global operator, which is constructed on the assumption that the source function varies linearly with the optical depth, is *almost* upper triangular. Although with Scharmer's global operator the number of iterations required to reach convergence may also be relatively small, the need to construct and to invert such an operator implies a computing time per iteration and a memory requirement that restricts its application to few-level RT in one-dimensional geometry. On the contrary, our SOR method does yield the very high convergence rate of a mathematically founded optimal *upper* triangular operator, with the ideal feature of a computing time and memory requirement per iteration as small as that of a *local* operator splitting method.

4.4. *Smoothing Capability*

As mentioned in the introduction, another method of interest for solving RT problems (mainly for two-dimensional and three-dimensional applications) is the *multigrid* method (Hackbush 1985), for which an essential part is the use of a basic iterative scheme capable of efficiently removing the high-frequency components of the error.

Our only purpose here is to demonstrate that our G-S method has comparatively excellent smoothing capabilities, which makes it the iterative method of choice for the *smoothing* part of multigrid RT codes. In order to illustrate this, we again

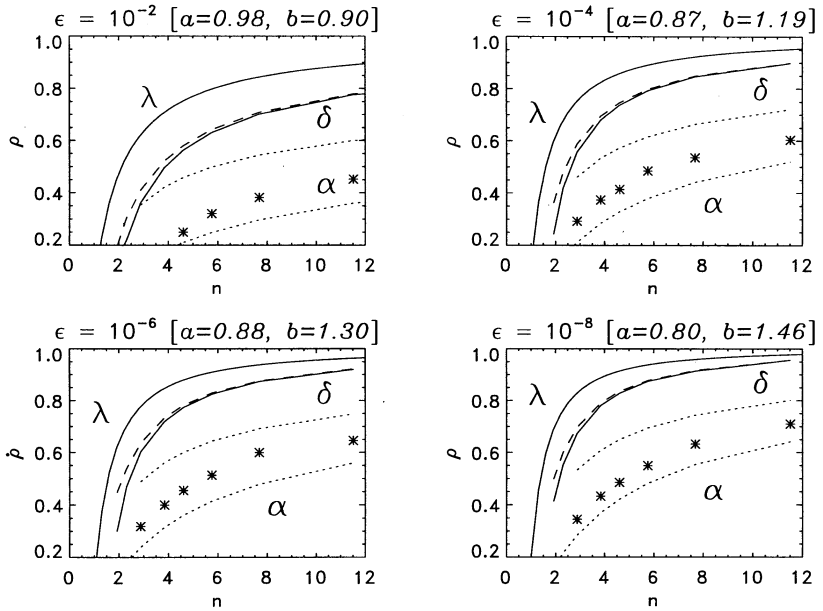

FIG. 8.—Same as in Fig. 4, but for the two-level atom line transfer case. The dashed line for δ is for the case in which the G-S process begins at the surface point, while the solid line for δ corresponds to the case in which the G-S process starts at the lower boundary point.

choose the coherent scattering problem for the case with $\epsilon = 10^{-6}$ and start the iterative calculation in a fine grid with nine points per decade with a highly fluctuating initialization whose error (calculated with respect to the fully converged solution in the grid used) is given in Figure 9*a*. Figure 9*b* shows that after 10 Jacobi iterations the high-frequency error components are still very significant. On the contrary, Figure 9*c* demonstrates that after only four G-S iterations, the remaining error is already very smooth. Additional information concerning the application and behavior of our G-S scheme in multigrid RT, both for two-level and multilevel atomic configurations, will be given in a future paper (for an advance report of some results, see Fabiani Bendicho et al. 1994).

5. CONCLUDING REMARKS

The RT methods developed in this paper have the ideal property of yielding the high convergence rates of *nonlocal* upper (or lower) triangular approximate operators, but with a memory requirement and a computing time per iteration similar to those of a *local* operator splitting technique. They neither require the actual construction of such *nonlocal* operators nor the application of any matrix inversion procedure. Therefore, they are also particularly suitable for multidimensional geometries.

In order to carry out RT calculations using our G-S and SOR iterative schemes, one has only to calculate the diagonal

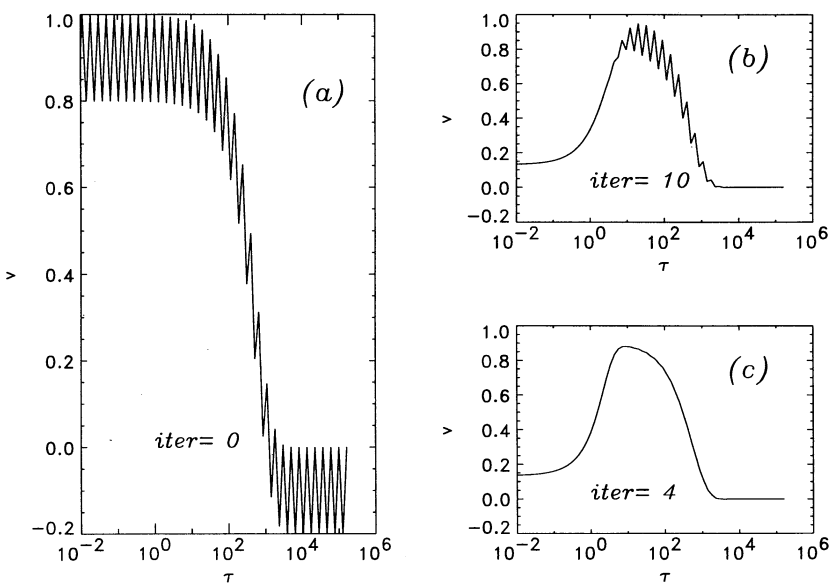

FIG. 9.—The variation with τ of the error in the chosen grid, i.e., of $v = S(n, \text{itr}) - S(n, \infty)$. The non-LTE parameter $\epsilon = 10^{-6}$, and $n = 9$. The v for itr = 0, i.e., the initialization error, is given in (*a*); (*b*) gives v after itr = 10 iterations with the optimal local operator method; (*c*) shows the error after iterating 4 times with our G-S scheme.

elements of the true Λ operator and to perform formal solutions of the transfer equation in a way similar to that explained in § 3. The novelty here lies in that the source function corrections are to be performed *within* the formal solution solver itself. One possibility is to do this as described in § 3, i.e., in a way such that each call to the formal solution solver produces as an output *one* G-S or *optimal* SOR iteration. However, it is important to point out that it is possible to develop still faster G-S-based methods. For instance, as we shall show in a forthcoming publication, one can achieve a factor 2 of additional improvement by using a modified formal solution solver such that each call to it produces as an output *two* truly G-S or SOR iterations: one after the *incoming* pass (with a convergence rate equivalent to that of a *lower* triangular approximate operator method) and the other iteration after the *outgoing* pass (with a convergence rate equivalent to that of an *upper* triangular approximate operator method).

Finally, we remark that the methods presented here are especially attractive because of their direct applicability to a variety of complicated RT problems of astrophysical interest. In future publications, we will show how these methods can be extended to the *nonlinear* multilevel atom case, to two- and three-dimensional geometries, and to the transfer of polarized radiation.

Some stages of this investigation were carried out while the authors were holding an ESA fellowship at the Dipartimento di Astronomia e Scienza dello Spazio (Florence University), and at the Kiepenheuer-Institut für Sonnenphysik (Freiburg). Partial support by the Spanish DGICYT (project PB 91-0530) and by the Regional Government of the Canary Islands (project PI 92/092) is also gratefully acknowledged. We thank the organizers of an informal workshop on multidimensional radiative transfer, which took place at Heidelberg University during 1994, for inviting us to present there the basic ideas contained in this paper. We are grateful to Egidio Landi Degl'Innocenti and Eduardo Simonneau for their careful reading of the manuscript. Thanks are also due to Monica Murphy for kindly checking the English. Last but not least, we should thank Larry Auer for having shared with us over the last few years his deep knowledge on numerical methods and radiative transfer.

REFERENCES

Auer, L. H. 1987, in Numerical Radiative Transfer, ed. W. Kalkofen (Cambridge: Cambridge Univ. Press), 101
———. 1991, in Stellar Atmospheres: Beyond Classical Models, ed. L. Crivellari, I. Hubeny, & D. G. Hummer (Dordrecht: Kluwer), 9
Auer, L. H., Fabiani Bendicho, P., & Trujillo Bueno, J. 1994, A&A, 292, 599
Auer, L. H., & Paletou, F. 1994, A&A, 285, 675
Cannon, C. J. 1973, ApJ, 185, 621
Carlsson, M. 1991, in Stellar Atmospheres: Beyond Classical Models, ed. L. Crivellari, I. Hubeny, & D. G. Hummer (Dordrecht: Kluwer), 39
Fabiani Bendicho, P., Trujillo Bueno, J., & Auer, L. H. 1994, in Proc. Workshop Numerical Methods for Multidimensional Radiative Transfer Problems, ed. R. Rannacher, S. Turek & R. Wehrse (Heidelberg: Univ. Heidelberg)
Hackbusch, W. 1985, Multi-Grid Methods and Applications (Berlin: Springer)
Hageman, L. A., & Young, D. M. 1981, Applied Iterative Methods (New York: Academic)
Hubeny, I. 1992, in Lecture Notes in Physics 401, The Atmospheres of Early-Type Stars, ed. U. Heber & C. S. Jeffrey (Berlin: Springer), 377
Jacobi, C. G. 1845, Astron. Nachr., 32, 297
Kahan, W. 1958, Ph.D. thesis, Univ. of Toronto
Kalkofen, W. 1987, in Numerical Radiative Transfer, ed. W. Kalkofen (Cambridge: Cambridge Univ. Press), 23
Klein, R. I., Castor, J. I., Greenbaum, A., Taylor, D., & Dykema, P. G. 1989, J. Quant. Spectrosc. Radiat. Transfer, 41, 199
Kunasz, P., & Auer, L. H. 1988, J. Quant. Spectrosc. Radiat. Transfer, 39, 67
Kunasz, P. B., & Olson, G. L. 1988, J. Quant. Spectrosc. Radiat. Transfer, 39, 1
Ng, K. C. 1974, J. Chem. Phys., 61, 2680
Mihalas, D. 1978, Stellar Atmospheres (New York: Freeman)
Olson, G. L., Auer, L. H., & Buchler, J. R. 1986, J. Quant. Spectrosc. Radiat. Transfer, 35, 431 (OAB)
Olson, G. L., & Kunasz, P. B. 1987, J. Quant. Spectrosc. Radiat. Transfer, 38, 325
Rybicki, G. B. 1991, in Stellar Atmospheres: Beyond Classical Models, ed. L. Crivellari, I. Hubeny, & D. G. Hummer (Dordrecht: Kluwer), 1
Rybicki, G. B., & Hummer, D. G. 1991, A&A, 245, 171
Scharmer, G. 1981, ApJ, 249, 720
Seidel, P. 1874, Münch Abh., 2 (3), 81
Steiner, O. 1991, A&A, 242, 290
Trujillo Bueno, J., Fabiani Bendicho, P. 1995, in preparation
Varga, R. S. 1962, Matrix Iterative Analysis (Englewood: Prentice-Hall)
Väth, H. M. 1994, A&A, 284, 319
Vinsome, P. K. W. 1976, in Proc. 4th Symp. on Numerical Simulation of Reservoir Performance of SPE of AIME, 140
Young, D. M. 1950, Ph.D. thesis, Harvard Univ.
———. 1971, Iterative Solution of Large Linear Systems (New York: Academic)
Young, D. M., & Gregory, R. T. 1972, A Survey of Numerical Mathematics, Vol. II (New York: Dover)