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Lambda-Acceleration: Convergence
Properties Using Exact Full and Diagonal
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Summary

We investigate the convergence properties of Λ -acceleration methods for non-LTE radiative transfer problems in planar and spherical geometry. Matrix elements of the “exact” Λ -operator are used to accelerate convergence to a solution in which both the radiative transfer and atomic rate equations are simultaneously satisfied. Convergence properties of 2-level and multilevel atomic systems are investigated for methods using: (i) the complete Λ -operator, and (ii) the diagonal of the Λ -operator. We find that the convergence properties for the method utilizing the complete Λ -operator are significantly better than those of the diagonal Λ -operator method, often reducing the number of iterations needed for convergence by a factor of between 2 and 7. However, the overall computational time required for large scale calculations — that is, those with many atomic levels and spatial zones — is typically a factor of a few larger for the complete Λ -operator method, suggesting that the approach should be restricted to problems in which convergence is especially difficult. In addition, we show that for problems with spherical symmetry the convergence properties found when using a Λ -operator based on contributions from only one hemisphere (thereby neglecting contributions from symmetry points) are only marginally worse than those when using the exact diagonal.

1. Introduction

Over the past decade, considerable progress has been made in developing numerical techniques for solving multilevel non-LTE (LTE \equiv local thermodynamic equilibrium) radiative transfer problems in astrophysics. Such problems are characterized by the requirement that multilevel atomic rate equations must be solved self-consistently with the radiation field. The fact that the radiation field can significantly affect the atomic level populations through photoexcitation and photoionization severely complicates the problem of modelling non-LTE plasmas. The methods of solution to this class of problems have relied on iterative techniques in which the level populations are “updated” until the equations of statistical equilibrium and radiative transfer are simultaneously satisfied. The manner in which the populations are updated has a significant effect on the rate of convergence and computational requirements of a problem.

Scharmer (1981, 1984) introduced a new approach to non-LTE radiative transfer based on Cannon’s operator perturbation technique (1973), in which he obtained approximate Λ -operators based on Rybicki’s core saturation assumption (1972) and the Eddington-Barbier relation. This method was later generalized to multilevel atomic systems and applied to stellar atmospheres by Scharmer and Carlsson (1985). Since that time a number of methods have been proposed to improve upon Scharmer’s technique.

Werner and Husfield (1985) proposed a method in which the contribution from the *diagonal* of the Λ -operator was used implicitly in the atomic rate equations. Approximate values of the diagonal Λ elements were obtained using the core saturation method with an adjustable parameter to specify the core-wing boundary of a line. Hamann (1986) applied this technique to spherically symmetric expanding stellar atmospheres. Olson, Auer, and Buchler (1986) also proposed a method utilizing the diagonal of the Λ -operator, but showed that using an accurate value for the diagonal was superior to using approximate diagonal elements. A similar conclusion was reached by Puls and Herrero (1988).

Olson and Kunasz (1987) showed that further improvements to the convergence rate in non-LTE radiative transfer problems can be obtained by using tridiagonal or pentadiagonal elements of the Λ -operator implicitly in the atomic rate equations. Unfortunately, the rate of convergence for banded Λ -operator methods (diagonal, tridiagonal, and pentadiagonal) deteriorates as the number of spatial grid zones increases (Olson and Kunasz 1987). This deterioration results from the fact that the plasma at each point along the computational grid can “communicate” a greater distance when the computational grid is relatively coarse. In an attempt to get around this problem Steiner (1991) proposed a multiple grid scheme in which coarse and fine spatial grids are alternatively used.

In this paper, we investigate the convergence properties of accelerated Λ -iteration techniques which utilize “exact” elements of either the complete or diagonal Λ -operator. Calculations are performed for both 2-level and multilevel atomic systems with planar and spherically symmetry. Accurate values for the elements of the Λ -matrix are computed using a computationally efficient technique recently proposed by Rybicki and Hummer (1991). We investigate the convergence rate and computational speed for both the complete and diagonal Λ -operator approaches. Results are presented showing the dependence of these properties on the number of spatial zones and atomic levels, and on whether Ng acceleration (1974; Auer 1987) is employed. In addition, for spherical systems we investigate whether convergence properties are significantly better when the exact diagonal elements of the Λ -operator are used; i.e., those which include contributions from points in opposite hemispheres.

When using the complete Λ -operator our approach is in some respects similar to those of Avrett and Loesser (1984, 1968) and Apruzese et al. (1980). The primary distinction between our study and previous work is that we use exact values of the Λ -operator which are obtained while using the differential form of the radiative transfer equation. That is, the Λ -matrix elements are calculated with the same coefficients of the tridiagonal matrix

operator used to solve the transfer equation. In addition, we examine the dependence of the convergence rate on the spatial grid, and make detailed comparisons with results using the diagonal Λ -operator approach in both planar and spherical coordinates. We emphasize the goal of this paper is not to argue that one Λ -acceleration approach is better than another for all problems. Rather, it is to compare Λ -acceleration approaches based on recent advances in numerical radiative transfer techniques, and to suggest that the complete Λ -operator method, because of its particularly good convergence properties, can be applied to non-LTE problems which exhibit convergence difficulties.

2. Calculation of Radiation Intensity and Λ -Matrix Elements

To calculate the radiation intensity we use the second-order form of the transfer equation. In planar geometry this can be written as (Mihalas 1978):

$$\left(1 - \mu^2 \frac{\partial^2}{\partial \tau_\nu^2}\right) u_{\mu\nu} = S_\nu, \quad (1)$$

where τ_ν is the optical depth at frequency ν measured along a ray normal to the slab boundary, μ is the direction cosine, and S_ν is the source function, which is assumed to be isotropic. The Feautrier variable $u_{\mu\nu}$ is defined as the average of the specific intensity $I_{\mu\nu}$ in the $\mu > 0$ and $\mu < 0$ directions:

$$u_{\mu\nu}(\tau_\nu) = \frac{1}{2}(I_\nu(\mu, \tau_\nu) + I_\nu(-\mu, \tau_\nu)). \quad (2)$$

The quantity u is readily evaluated along an optical depth grid at each angle and frequency point by solving a tridiagonal system of equations. In the calculations described below, second-order accurate boundary conditions are used at the “top” of the atmosphere where we assume no incident radiation:

$$I_\nu(\tau_\nu = 0, -\mu) = 0.$$

The matrix elements of the Λ -operator are calculated using the method recently proposed by Rybicki and Hummer (1991). The Λ -operator can be expressed by the relation:

$$u_{\mu\nu} = \Lambda_{\mu\nu}[S_\nu], \quad (3)$$

where $\Lambda_{\mu\nu}$ is a matrix of size $N_D \times N_D$, where N_D is defined as the number of optical depth points. Let T be a differential operator defined by Eq. (1), so that:

$$T_{\mu\nu}u_{\mu\nu} = S_\nu. \quad (4)$$

The quantity T is an $N_D \times N_D$ tridiagonal matrix. Combining Eqs. (3) and (4) gives

$$T_{\mu\nu}\Lambda_{\mu\nu} = 1. \quad (5)$$

Rybicki and Hummer (1991) showed that all diagonal elements of the “true” (or exact) Λ -operator can be quickly found in $\sim N_D$ operations. Little extra computational effort is required beyond that expended to evaluate the radiation intensity. In addition, the off-diagonal elements are obtained from simple recursion relations.

In spherical geometry the form of the transfer equation is similar to that for the planar case (Eq. (1)). However, in this case the angle-dependent information is obtained by evaluating the transfer equation along a grid of rays with impact parameters defined by the radial mesh (see e.g., Mihalas, Kunasz, and Hummer 1975), as illustrated in Fig. 1. A significant difference between planar and spherical geometries is that in spherical coordinates a single ray can intersect the same spatial zone of the computational grid more than once. For instance, two points from the same zone, points A and B in Fig. 1, are intersected by the ray defined by impact parameter P. Because of this, the diagonal elements — as well as off-diagonal elements — of the Λ -operator depend not only on the photons emitted on the observer side of the sphere (point A), but also on the photons emitted from the symmetry point in the opposite hemisphere (point B). A reflective boundary condition at the plane of symmetry cannot be used to obtain the photoexcitation rate at point A caused by

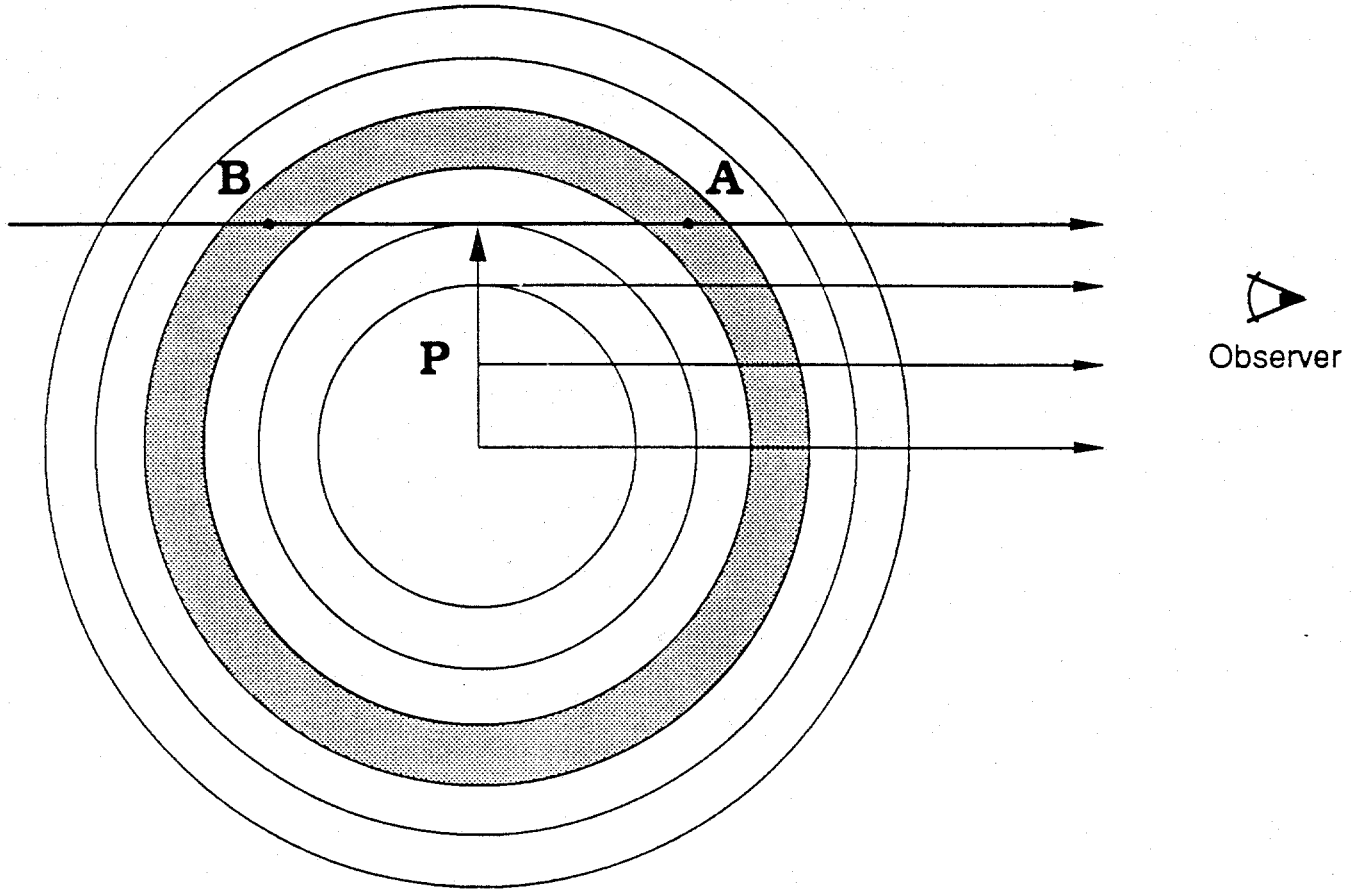


Figure 1. Illustration of spatial grid used to solve the radiative transfer equation in spherical coordinates. The ray defined by impact parameter P intersects the same zone at points A and B .

photons emitted at point B because one must consider the effects of attenuation between points A and B. Below, we also investigate whether using the contribution from only one of the hemispheres to the lambda operator leads to any significant degradation in the rate of convergence in spherical radiative transfer problems.

3. Atomic Rate Equations

A good understanding of different Λ -acceleration techniques can best be attained by examining the case of a 2-level atom. The steady-state rate equation for a system with 2 bound states can be written as (Mihalas 1978):

$$S_L = (1 - \varepsilon)\bar{J} + \varepsilon B_\nu, \quad (6)$$

where the mean intensity is

$$\bar{J} \equiv \int_0^\infty d\nu \phi_\nu J_\nu = \int_0^\infty d\nu \phi_\nu \int_0^1 d\mu u_{\mu\nu}, \quad (7)$$

S_L is the line source function, ε is the thermalization parameter, B_ν is the Planck function at the transition frequency ν , and ϕ_ν is the line profile. For convenience, we have neglected in Eq. (6) the effects of a background continuum. We also assume complete frequency redistribution. The monochromatic mean intensity at a point a along the computational grid is related to the Λ -operator by

$$\bar{J}(\tau^a) = \sum_{e=1}^{N_D} \bar{\Lambda}^{ea} S_L^e, \quad a = 1, \dots, N_D, \quad (8)$$

where

$$\bar{\Lambda}^{ea} = \int_0^\infty d\nu \phi_\nu \Lambda_\nu^{ea} = \int_0^\infty d\nu \phi_\nu \int_0^1 d\mu \Lambda_{\mu\nu},$$

and the summation is over all optical depth points. The superscripts in Eq. (8) represent points of emission (e) and absorption (a). Substituting Eq. (8) into Eq. (6) we obtain

$$S_L^a - (1 - \varepsilon) \sum_{e=1}^{N_D} \bar{\Lambda}^{ea} S_L^e = \varepsilon B_\nu. \quad (9)$$

The matrix elements of the Λ -operator are determined during the solution to the radiative transfer equation. Since they are a nonlinear function of the source function (and atomic level populations), the self-consistent solution of S and Λ is obtained by iteration.

The most straightforward way to calculate S at a new iteration cycle k is to use the value of the radiation field computed using the source function from the previous iteration, $k - 1$. Then

$$S_L^a(k) = \varepsilon B_\nu + (1 - \varepsilon) \sum_{e=1}^{N_D} \bar{\Lambda}^{ea} S_L^e(k - 1). \quad (10)$$

This approach is referred to as Λ -iteration, a method whose convergence problems are well known (see e.g., Mihalas 1978).

A technique with significantly better convergence properties is the diagonal Λ -operator method (Werner and Husfield 1985; Olson et al. 1986). In this approach, the source function is evaluated using the term containing the diagonal of the Λ -operator *implicitly* in the rate equation. This leads to

$$\begin{aligned} S_L^a(k) &= \frac{\varepsilon B_\nu + (1 - \varepsilon) \sum_{e \neq a} \bar{\Lambda}^{ea} S_L^e(k - 1)}{1 - (1 - \varepsilon) \bar{\Lambda}^{aa}} \\ &= \frac{\varepsilon B_\nu + (1 - \varepsilon) (\bar{J}(k - 1) - \bar{\Lambda}^{aa} S_L(k - 1))}{1 - (1 - \varepsilon) \bar{\Lambda}^{aa}}. \end{aligned} \quad (11)$$

Note that in evaluating the summation in Eq. (11) only the diagonal of the Λ -operator needs to be computed. The reason for the better convergence properties is that the “net” mean intensity, $\bar{J} - \bar{\Lambda} S_L$, effectively discounts the effects of scattering in the optically thick cores of lines. Formulation of the rate equation for using the tridiagonal and pentadiagonal parts of the Λ -operator is straightforward. However, a degradation in the convergence properties is observed as the number of optical depth points increases (Olson and Kunasz 1987).

A significant improvement in convergence properties can be realized by using the complete Λ -operator (all elements of the matrix) implicitly in the rate equations. The rate

equation can then be expressed as

$$S_L^a(k)(1 - (1 - \varepsilon)\bar{\Lambda}^{aa}) - (1 - \varepsilon) \sum_{e \neq a} \bar{\Lambda}^{ea} S_L^e(k) = \varepsilon B_\nu, \quad a = 1, \dots, N_D. \quad (12)$$

The source function distribution for a 2-level atom is then obtained by inverting an $N_D \times N_D$ matrix. The improved rate of convergence stems from the fact that at each point in the atmosphere the contribution to the radiation field from all of the other points is monitored. The photoexcitation rate in a given spatial zone (a) due to photons emitted in a different zone (e) is proportional to the source function of the emitting zone. By solving the rate equations for all the zones simultaneously, the convergence number of iterations required to get a self-consistent solution of the radiative transfer and atomic rate equations can be significantly reduced.

The main drawback to using the complete Λ -operator for large scale calculations with many atomic levels and optical depth points is that the size of the matrix is $(N_L \cdot N_D) \times (N_L \cdot N_D)$, where N_L is the number of atomic levels. However, since in most calculations atomic levels of a given ionization stage are allowed to undergo transitions only to levels either within the same ion or adjacent ionization stages, the matrix is banded. The band width is $\sim N_L^* \cdot N_D$, where N_L^* is the maximum number of levels in a given stage of ionization. For banded matrices the number of operations scales as nm^2 ($n \equiv$ order of the matrix, $m \equiv$ band width), whereas for full matrices the number of operations scales as n^3 (Dongarra et al. 1979). One can also take advantage of the banded structure to reduce core memory requirements.

For multilevel atomic systems, the steady-state rate equation for level i is:

$$\frac{dn_i}{dt} = -n_i \sum_{j \neq i}^{N_L} W_{ij} + \sum_{j \neq i}^{N_L} n_j W_{ji} = 0, \quad (13)$$

where W_{ij} and W_{ji} are the depopulating and populating rates between levels i and j . For upward transitions ($i < j$):

$$W_{ij} = B_{ij} \bar{J}_{ij} + n_e C_{ij} + n_e \gamma_{ij} + \beta_{ij} \quad (14)$$

while for downward transitions ($i > j$):

$$W_{ij} = A_{ij} + B_{ij}\bar{J}_{ij} + n_e D_{ij} + n_e \alpha_{ij} + n_e^2 \delta_{ij}, \quad (15)$$

where n_e is the electron density, A_{ij} and B_{ij} are the Einstein coefficients for spontaneous emission and stimulated emission and absorption, C_{ij} and D_{ij} are the collisional excitation and deexcitation rate coefficients, α_{ij} represents the sum of the radiative and dielectronic recombination rate coefficients, β_{ij} is the photoionization rate, and γ_{ij} and δ_{ij} are the rate coefficients for collisional ionization and recombination.

In the complete Λ -operator formalism, the stimulated absorption and emission rates are written in terms of the Λ -matrix elements:

$$n_j^a B_{ji} \bar{J}_{ij} - n_i^a B_{ij} \bar{J}_{ij} = \begin{cases} -A_{ji} \sum_{e=1}^{N_D} n_j^e \bar{\Lambda}_{ji}^{ea} (N_j^a S_L^e / N_j^e S_L^a) & (i < j) \\ A_{ij} \sum_{e=1}^{N_D} n_i^e \bar{\Lambda}_{ij}^{ea} (N_i^a S_L^e / N_i^e S_L^a) & (i > j), \end{cases} \quad (16)$$

where N_j^a represents the total number of atoms in state j and optical depth zone a . Equations (13) and (16) represent a set of $N_L \cdot N_D$ coupled rate equations. As stated earlier, the grand matrix becomes banded when transitions are restricted to take place between adjacent ions.

The photoionization rate can be written as

$$n_i R_{i\kappa} = \sum_{e=1}^{N_D} \int_{\nu_1}^{\infty} d\nu \frac{4\pi}{h\nu} \alpha_\nu^a \Lambda_\nu^{ea} \frac{B_\nu^\dagger}{b_1}, \quad (17)$$

where α_ν^a is the photoionization cross section for the absorbing point a . Both B_ν^\dagger and b_1 are evaluated at the emission point e . They are defined as:

$$B_\nu^\dagger = \frac{(2h\nu^3/c^2)}{e^{h\nu/kT} - b_1^{-1}}, \quad (18)$$

and

$$b_1 = \left(\frac{n_i}{n_\kappa} \right) / \left(\frac{n_i}{n_\kappa} \right)^*. \quad (19)$$

The population densities of the lower level and upper continuum state are represented by n_i and n_κ , respectively. The asterisk in Eq. (20) signifies the LTE ratio for the populations.

4. Results for 2-level and Multilevel Atomic Systems

We have performed a series of 2-level and multilevel atom calculations in both planar and spherical geometries to investigate the potential benefits of using the diagonal or complete matrix of the exact Λ -operator to accelerate convergence. The purpose of calculations is to study the trade-offs in the rate of convergence and computational speed using the complete and diagonal Λ -operator methods. In addition, we examine for problems with spherical symmetry the extent to which neglecting the contribution from symmetry points to the diagonal Λ -operator affects the convergence rate. The motivation for this comes from previous studies which showed that the convergence rate improves as more accurate values of the Λ -operator are used in the atomic rate equations (Olson et al. 1976; Puls and Herrero 1988).

The method of solution is as follows. We start with LTE population distributions. The radiation intensity is obtained from formal solutions to the transfer equation. We calculate the Λ -matrix elements utilizing the same coefficients of the tridiagonal matrix operator from which the intensity is computed. New populations are obtained by solving the atomic rate equations using all, part, or none (Λ -iteration) of the Λ -operator. Iteration continues until the maximum relative change in the population densities at iteration cycle k ,

$$\Delta_{\max}(k) \equiv \max \left[\frac{n_{i,d}(k) - n_{i,d}(k-1)}{n_{i,d}(k-1)} \right], \quad i = 1, \dots, N_L; \quad d = 1, \dots, N_D \quad (20)$$

falls below some specified criterion.

We performed calculations both with and without Ng acceleration (Auer 1987; Ng 1974). A modest effort was made to determine the optimum parameter for applying this technique. We found for multilevel atom calculations using the *diagonal* Λ -operator approach that fourth-order Ng acceleration applied every 6th iteration generally works best, while the second-order method applied every 4th iteration works best for the *complete* Λ -operator approach. In the 2-level atom calculations, the second-order method was used.

4.1. Two-level Atom Calculations

In the first series of calculations, we examine the dependence of the convergence rate on: (i) the type of Λ -acceleration scheme used, and (ii) the number of optical depth points in the spatial grid. We assumed a Doppler line profile with a total optical depth of $T = 10^4$, and a thermalization parameter of $\varepsilon = 10^{-4}$. Each calculation was performed for planar geometry. The number of zones in the optical depth grid was varied between 24 (about 2 points per decade) and 72 (about 6 points per decade).

Figure 2 shows the maximum relative change in population as a function of the iteration cycle for calculations with 24 optical depth points. The 3 curves represent the results from calculations using the complete Λ -matrix (solid curve), the diagonal of the Λ -matrix (dotted curve), and Λ -iteration (dot-dashed curve). It is clear that the convergence rate using the complete Λ -operator implicitly in the rate equations is significantly better than both the diagonal Λ and Λ -iteration methods. It takes 28 iterations to reach a Δ_{\max} of 10^{-3} for the diagonal operator approach while it takes only 4 iterations using the full Λ -operator approach. It also takes approximately 7 times as many iterations for the diagonal method when a lower criterion of 10^{-5} is used (40 iterations versus 6 iterations). Figure 2 also shows that Δ_{\max} for the diagonal method exceeds that for Λ -iteration during the first 18 cycles. This is simply an artifact of the populations moving faster toward the correct solution in the diagonal method. In later cycles, Δ_{\max} is less because the source function distribution is near the final solution.

A similar effect is seen in Fig. 3, where the results are shown for an identical set of calculations, but with $N_D = 72$ points. In this case it takes 50 cycles for the diagonal operator method to reach a Δ_{\max} of 10^{-2} . On the other hand, the method utilizing the full Λ -operator shows approximately the same rate of convergence as in the $N_D = 24$ zone calculation, with $\Delta_{\max} \approx 10^{-3}$ after 4 cycles and $\Delta_{\max} \approx 10^{-5}$ after 7 cycles. The reason for the observed independence of the number of grid points is that information regarding where

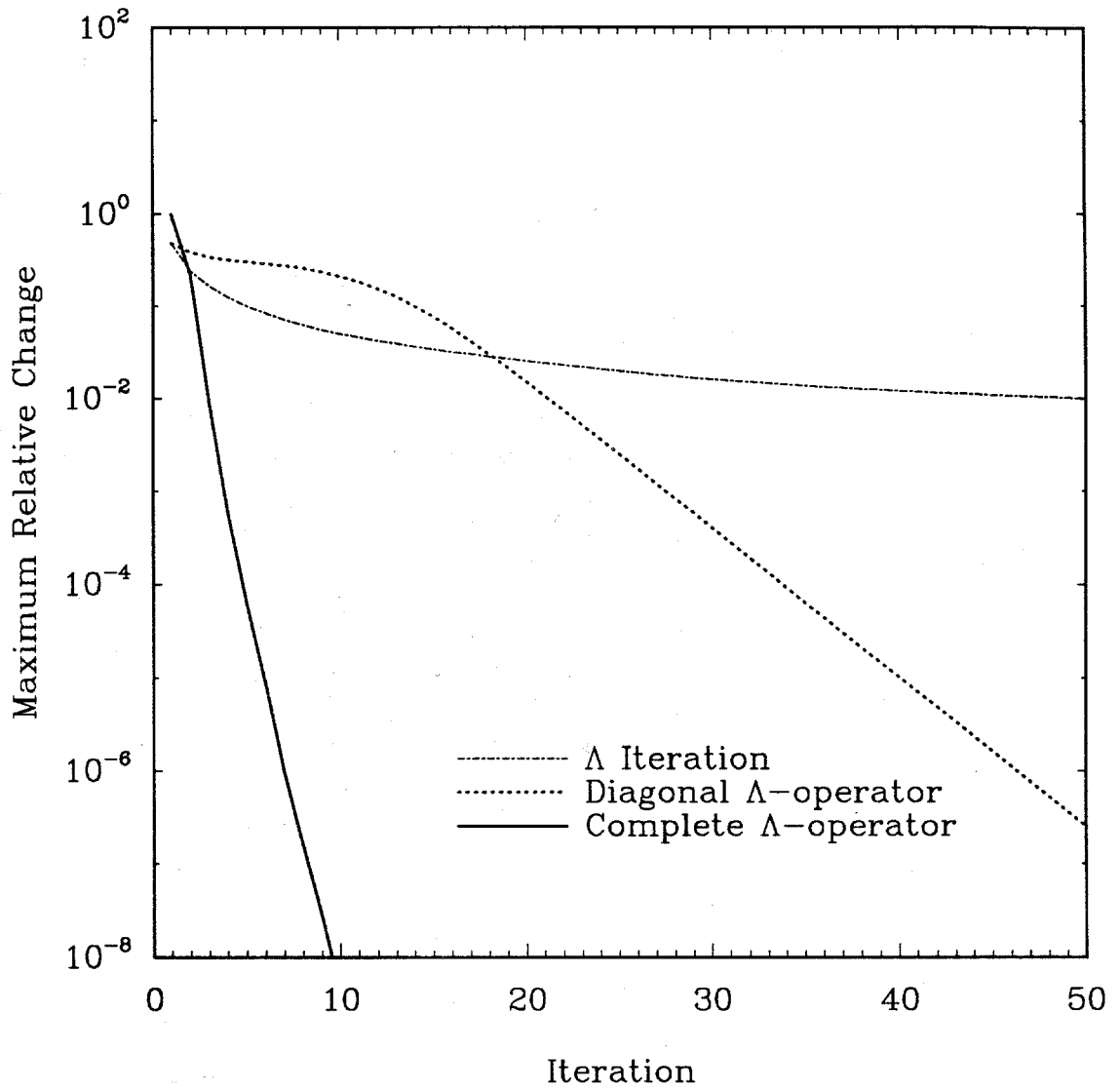


Figure 2. Maximum relative change in the population densities between successive iterations for planar calculation with $N_D = 24$ zones, $T = 10^4$, and $\varepsilon = 10^{-4}$.

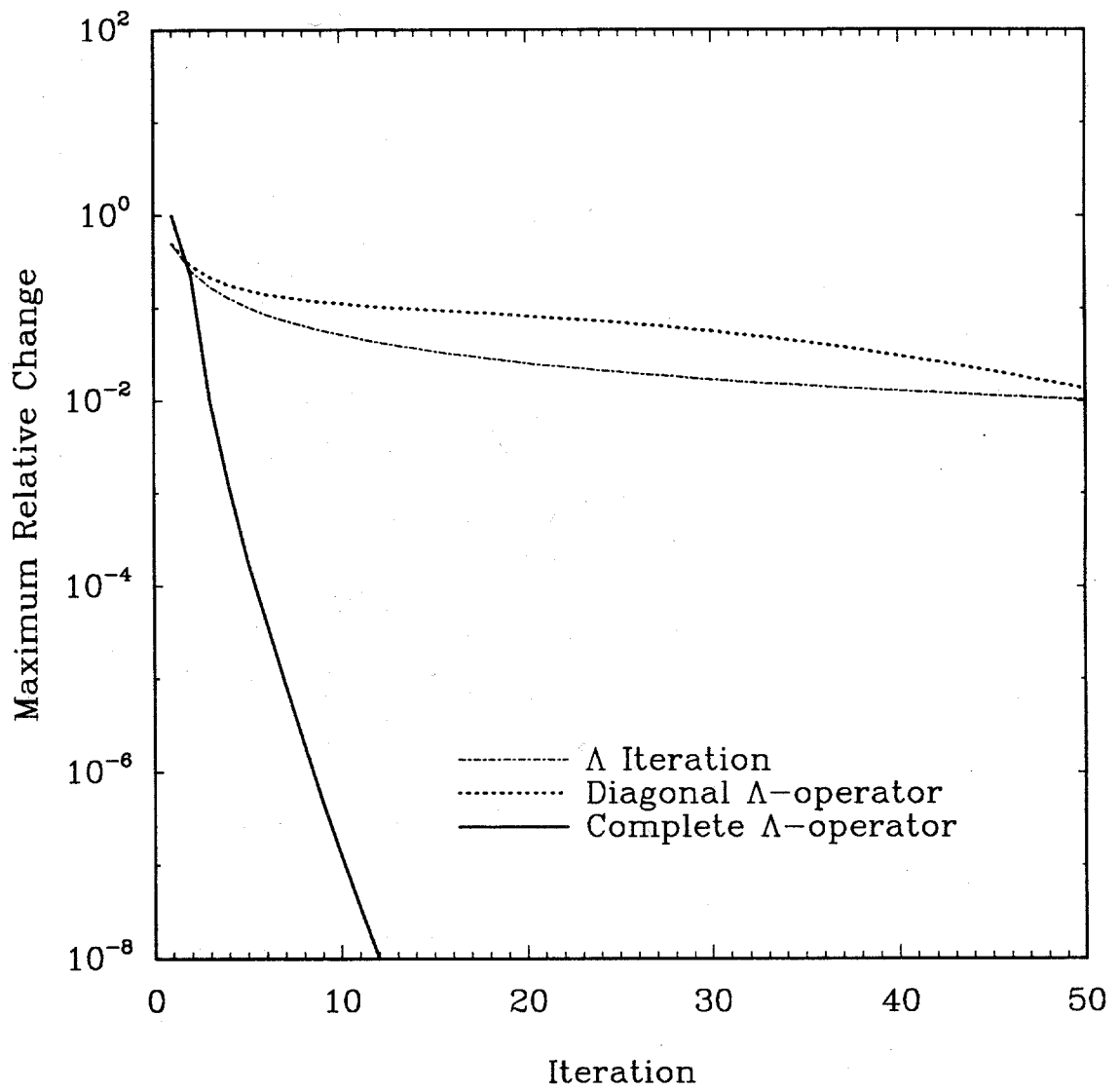


Figure 3. Maximum relative change in the population densities between successive iterations for planar calculation with $N_D = 72$ zones, $T = 10^4$, and $\varepsilon = 10^{-4}$.

photons originate in the atmosphere is not lost as the space between grid points decreases in the full Λ -operator approach. Each point in the atmosphere “sees” all other points in the atmosphere regardless of the number of points. This is not the case for the diagonal Λ -operator method. In this case each point sees only photons that originate locally (i.e., in the same zone).

Figure 4 shows results for a series of calculations in which Ng acceleration was applied every fourth cycle. With the exception of employing Ng acceleration, the calculations are identical to those shown in Fig. 3. Note that the rate of convergence improves for all 3 methods. This is especially obvious for the Λ -iteration and diagonal operator methods where Ng acceleration has been applied many times (compare with Fig. 3). In this case $\Delta_{\max} \approx 10^{-3}$ and 10^{-5} after about 24 and 40 cycles, respectively, for the diagonal Λ -operator method. This represents approximately 6 times as many cycles as the full Λ -operator case.

In previous investigations (Olson et al. (1986); Puls and Herraro (1988)) it was shown that calculating “accurate” values for the diagonal Λ -operator results in better convergence properties compared to when using “approximate” Λ -operators. In spherical geometry, however, exact values for the diagonal elements of the Λ -operator are somewhat more difficult to obtain. This is because a ray can intersect the same spherical surface at 2 points. There are thus 2 contributions to each element of the diagonal: the “self-coupling” or “local” contribution (point A, Fig. 1) and a “non-local” contribution (point B) for which the attenuation effects between points A and B must be considered. It is straightforward to calculate the non-local contribution using the recursion relations referred to in Section 2. However, this calculation takes a non-trivial amount of computer time. If most of the off-diagonal information is then being discarded, as it is for the diagonal Λ -operator method, it may be advantageous to neglect the non-local contribution. The following question arises: to what extent is the convergence improved by considering the non-local contribution to the diagonal Λ -operator?

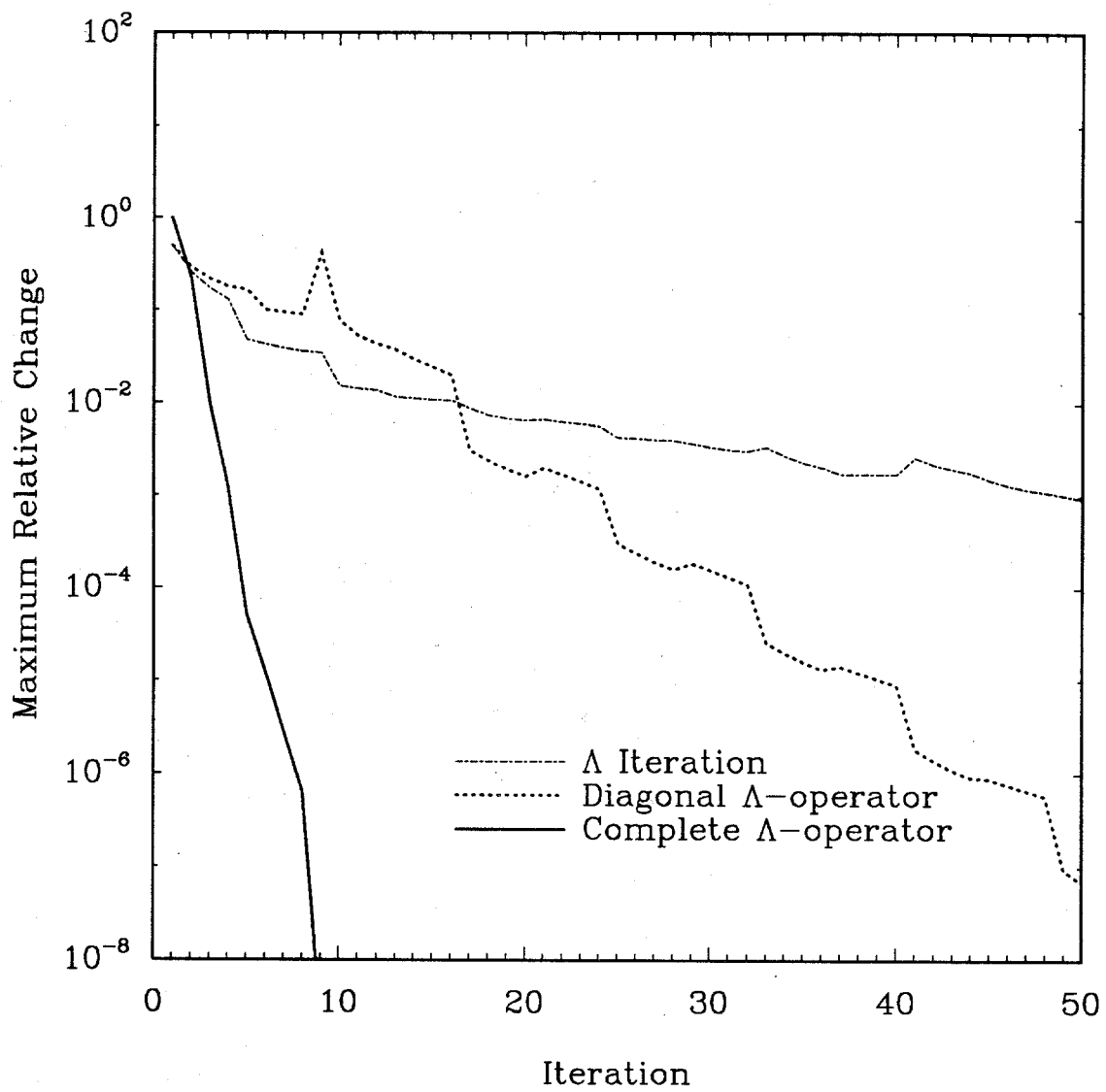


Figure 4. Same as Figure 3, but for calculations with Ng acceleration applied every fourth iteration.

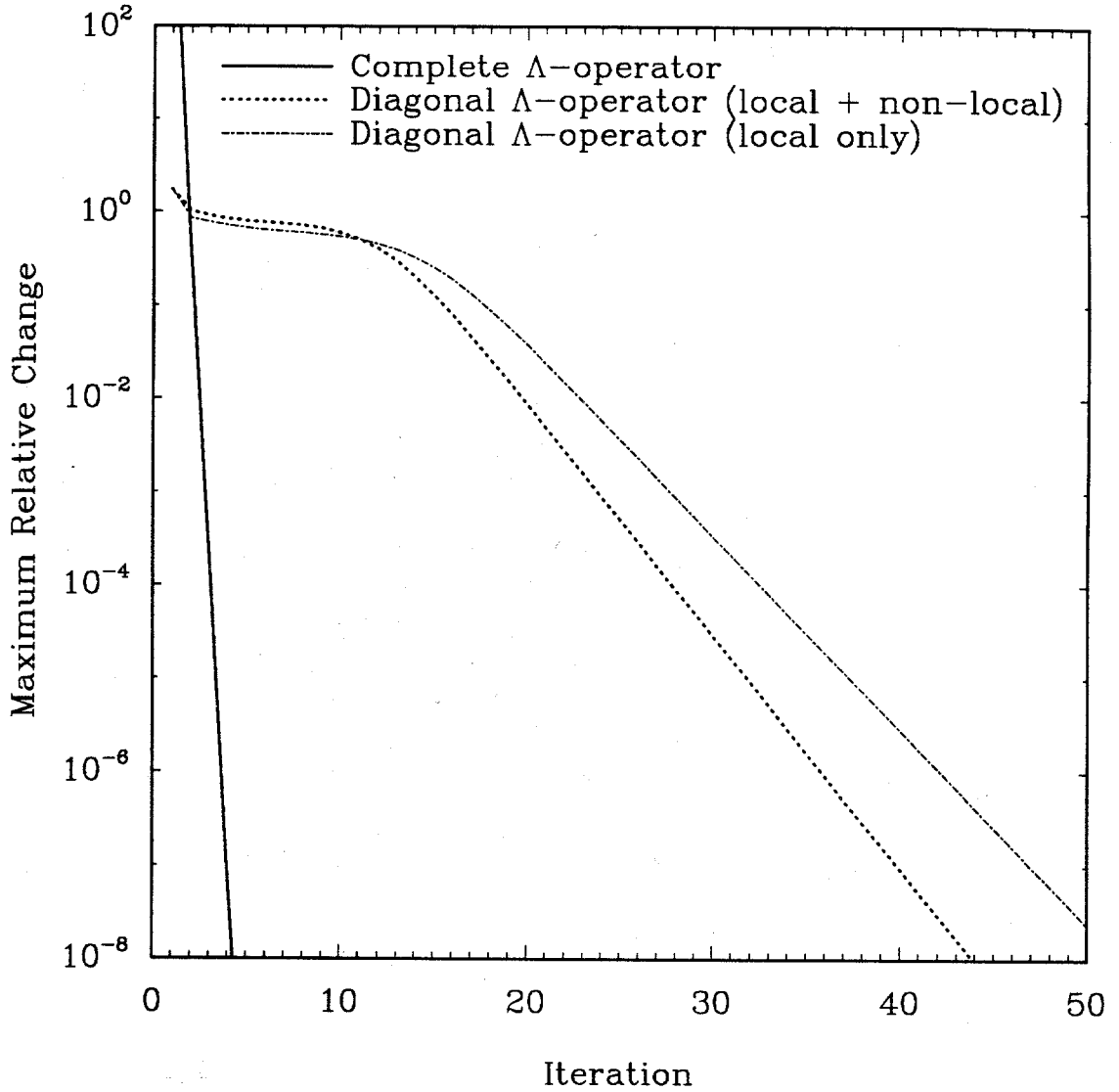


Figure 5. Maximum relative change in the population densities between successive iterations for spherical calculation with $N_D = 24$ zones, $T = 10^1$, and $\varepsilon = 10^{-4}$. Results are compared for diagonal operator methods using the exact lambda-operator (“local” + “non-local” case) and an approximation for the diagonal in which only local contributions are considered.

Figure 5 shows the convergence properties for full and diagonal Λ -operator calculations with $T = 10^1$ and $\varepsilon = 10^{-4}$. Note that for these conditions the photon thermalization depth ($\Lambda \sim \varepsilon^{-1/2}$) exceeds the total optical depth, so that most photons can scatter throughout the sphere before being destroyed. Thus, the non-local contribution to the Λ -operator will be relatively large as compared to lines which are effectively thick. Results are shown for two diagonal Λ -operator cases. In the case represented by the dotted curve, the non-local contribution to the diagonal was included. In the other (dot-dashed curve) only the local contribution was considered. The solid curve represents results using the complete Λ -operator, where again we find extremely rapid convergence.

It is seen in Fig. 5 that by neglecting the non-local contribution to the diagonal Λ -operator, the number of iterations required increases by only about 15 to 20%. Calculations performed for an effectively thick line, with $T = 10^4$ and $\varepsilon = 10^{-4}$, showed virtually no difference in the convergence rate between the two calculations. Our results thus indicate that there is only a modest improvement when using the exact diagonal Λ -operator in spherical geometry, and that computing the diagonal using only the local contribution will result in a net savings in computer time.

4.2. Multilevel Atom Calculations

We next present results from multilevel atom calculations in planar and spherical geometries using diagonal and complete Λ -operators. Our aim is to compare convergence properties and computer time requirements for the diagonal and complete Λ -operator methods. Calculations were performed for He atoms with 12 levels distributed over 3 ionization stages ($N_{HeI} = 1$, $N_{HeII} = 10$, and $N_{HeIII} = 1$). In each calculation, the temperature was 30,000 K, and the electron and ion density were both 10^{10} cm^{-3} . The slab width in the planar calculations and the radius for spherical calculations were both 10^8 cm . For these conditions the maximum line optical depth (Doppler profile assumed) was $\sim 10^4$ and the continuum optical depth was $\sim 10^1$.

Table 1. Timing Results from Planar Multilevel Calculations*Diagonal Λ -Operator Method*

| N_D | Iterations | CPU Time (s) |
|-------|------------|--------------|
| 20 | 12 | 1.1 |
| 40 | 17 | 2.8 |
| 80 | 21 | 6.7 |

Complete Λ -Operator Method

| N_D | Iterations | CPU Time (s) |
|-------|------------|--------------|
| 20 | 9 | 1.9 |
| 40 | 9 | 8.3 |
| 80 | 10 | 47 |

In each case the radiation field was computed at 10 frequency points per transition. The number of angle grid points was 2 for planar calculations and $N_D + 5$ for spherical calculations. The calculations were performed on the CRAY Y-MP at the San Diego Supercomputer Center using a moderately-vectorized version of our radiative transfer code. To compute the level populations, we performed matrix inversions with vectorized versions of the LINPACK linear algebra routines (Dongarra et al., 1979). Iteration continued until Δ_{\max} fell below 10^{-3} . In all cases, Ng acceleration was applied.

Tables 1 and 2 show timing results from planar and spherical calculations, respectively. For each geometry and Λ -operator method, we performed calculations using 20, 40, and 80 optical depth points. In all cases the CPU time required for the diagonal Λ -operator method was less than that required for the corresponding complete Λ -operator calculation. In the

Table 2. Timing Results from Spherical Multilevel Calculations*Diagonal Λ -Operator Method*

| N_D | Iterations | CPU Time (s) |
|-------|------------|--------------|
| 20 | 19 | 3.0 |
| 40 | 25 | 13 |
| 80 | 37 | 68 |

Complete Λ -Operator Method

| N_D | Iterations | CPU Time (s) |
|-------|------------|--------------|
| 20 | 9 | 4.0 |
| 40 | 9 | 21 |
| 80 | 7 | 103 |

spherical geometry calculations the CPU ratio for the two methods shows little dependence on the number of points in the spatial grid, with t (complete- Λ)/ t (diagonal- Λ) ranging from 1.3 to 1.6. On the other hand, this ratio shows a fairly strong dependence on N_D in the planar calculations, ranging from 1.7 in the $N_D = 20$ calculation to 7 in the $N_D = 80$ calculation. The reason for the stronger dependence of N_D in the planar case is that a larger fraction of the CPU time is spent on inverting the grand matrix for the rate equations. Relatively little time is required to compute the radiation intensity and the Λ -matrix elements because the computer code is readily vectorized over both frequency and angle. In spherical geometry, vectorization over angle is difficult because the number of optical depth points varies for each angle point (which is defined by the impact parameter). In addition, more angle points are generally used in spherical calculations. Because of this, calculation of the intensity and Λ -operator consumes a substantial amount of CPU time. Thus, in spherical

geometry there does not appear to be an enormous difference in the computational requirements between the complete and diagonal Λ -operator methods. Nonetheless, for radiative transfer problems in which convergence is not particularly difficult, the diagonal Λ -operator method appears to be the best approach.

It is also seen in Tables 1 and 2 that the number of iterations required for convergence shows little dependence on the number of optical depth points. This was also observed to be the case in the 2-level atom calculations. It is for this reason that the total CPU time in spherical geometry calculations using the complete Λ -operator method can be less than a factor of 2 greater than the diagonal case. By comparison, the CPU time *per iteration* is about 8 times greater in the $N_D = 80$ case.

It is clear from this investigation that both of the Λ -acceleration techniques we have studied offer distinct advantages. In all cases we have examined, the diagonal Λ -operator approach needed less CPU time (and memory) to converge to a solution. The advantage of the complete Λ -operator technique is that it has very good convergence properties. In fact, experience has shown that in several problems in which convergence is either not attained or is particularly slow using the diagonal Λ -operator, convergence is quickly attained with the complete Λ -operator method. We cite as one example the spherical multilevel calculation with 80 depth points. It was found that the number of iterations required to reach $\Delta_{\max} = 10^{-3}$ depended somewhat sensitively on the Ng acceleration parameters: 37 iterations for fourth-order acceleration every 6th cycle, but 84 iterations for second-order acceleration every 4th cycle. In fact, in the latter case, the overall CPU time was greater for the diagonal Λ -operator calculation than the complete Λ -operator calculation. As a rule of thumb, we have found that in problems where the diagonal method fails, the complete Λ -operator approach can often, though not always, succeed. We find that a particularly troublesome class of problems for both methods is when the electron density distribution

is significantly affected by photoionizations. This appears to be similar to the problem described by Hummer and Voels (1988) for O stars with high helium abundance.

5. Summary and Discussion

We have studied the convergence properties of Λ -acceleration techniques which utilize either part or all of the exact Λ -operator. Accurate values of the Λ -matrix elements were obtained in a manner consistent with the differential form of the transfer equation. Results using the complete Λ -operator implicitly in the atomic rate equations were compared with those for which only the diagonal elements of the Λ -operator were used. We have presented results from 2-level and multilevel atom radiative transfer calculations in planar and spherical geometries.

Our results indicate that the number of iterations required to obtain converged solutions with the complete Λ -operator method is typically a factor of between 2 and 6 fewer than with the diagonal Λ -operator method. We also find that the rate of convergence in the complete Λ -operator method shows little dependence on the number of spatial grid points, whereas the convergence properties worsen as the grid spacing decreases when only the diagonal elements are used. On the other hand, the overall computational time required was found to be less with the diagonal method by a factor of between 1.3 and 7. The benefits in reduced computer times tended to be greater in the planar calculations where vectorization over angle and frequency can be readily performed and the number of angle points can be considerably less. Therefore, in radiative transfer problems in which convergence is easily attained the diagonal Λ -operator appears to be the more computationally efficient approach.

Although the diagonal Λ -operator approach has some significant advantages, the complete Λ -operator technique may be a useful tool for calculations in which convergence is a problem. Our experience in using the complete Λ -operator method suggests that it should be applied to radiative transfer problems in which convergence either occurs very slowly or is unattainable. In our efforts to develop codes to study radiative transfer in both

astrophysical and laboratory plasmas (see e.g., MacFarlane et al. (1990,1991)) there have been several instances in which the diagonal approach failed, while the complete Λ -operator method was successful in achieving a converged solution. It might also be interesting to apply this approach to calculations with partial redistribution, which evidently can also exhibit convergence difficulties.

The main drawback to the complete Λ -operator approach is that it puts greater demands on computer time and memory. The simultaneous solution of the atomic rate equations for all levels at all optical depth points requires the inversion of a single matrix of size as high as $(N_L \cdot N_D) \times (N_L \cdot N_D)$ (see e.g., Werner and Husfield 1985). However, one can significantly reduce the computational requirements by taking advantage of the fact that transitions occur only between adjacent ionization stages. By arranging the grand matrix such that there are $N_L \times N_L$ submatrices of size $N_D \times N_D$, the band width of the grand matrix is $\sim N_D$ times the maximum number of excitation states in an ion. This approach can lead to a substantial reduction in both computer time and memory, and can make an otherwise computationally prohibitive problem quite tractable.

We have also investigated for spherical systems the degree to which the rate of convergence degrades when the “non-local” contribution (that arising from symmetry points in the opposite hemisphere) to the diagonal Λ -operator is neglected. Here, it was found that the convergence rate worsens only slightly, with the number of iterations being the same in effectively thick calculations, and increasing by $\sim 20\%$ in effectively thin calculations. Thus, there appears to be little benefit in including non-local contributions when computing the diagonal Λ -operator.

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