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An operator splitting method for atmospheres with shocks

B. Buchholz[1], **P.H. Hauschildt**[2], **W. Rammacher**[1], **P. Ulmschneider**[1]

[1] Institut für Theoretische Astrophysik der Universität Heidelberg, Im Neuenheimer Feld 561, D-69120 Heidelberg, Germany
[2] Arizona State University, Department of Physics and Astronomy, BOX 871504, Tempe, AZ 85287-1504, USA

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Abstract. We develop a fast operator splitting (OS) method to solve spectral line radiative transfer problems in time-dependent hydrodynamic computations with shock discontinuities, assuming complete redistribution. The convergence properties and the results obtained with our method are compared with results obtained using a modified core-saturation method and with the Λ-iteration. We find that our operator splitting method is robust, accurate and fast.

Key words: radiative transfer – numerical methods – sun: chromosphere – shock waves

1. Introduction

The numerical treatment of spectral line radiation transport in the presence of shock discontinuities is difficult and requires an efficient method of solution. Moreover, in time-dependent calculations of stellar chromospheres or coronae, line transfer problems have to be solved several *thousand* times during a typical simulation. Therefore, it is essential to have a robust and fast, but still reasonably accurate method. We call a method robust, if it works reliably even under extreme conditions, e.g., when shocks closely approach regular grid-points, or when shocks overtake other shocks, leading to large differences in optical depth between adjacent grid-points.

In principle, the core-saturation method developed by Kalkofen & Ulmschneider (1984) fulfills these requirements: it is robust as well as fast, and it is able to treat shocks of arbitrary strength. Perhaps the most severe numerical problem of the core-saturation method is that its convergence properties depend *critically* on an optical depth parameter $\Delta\tau_\gamma$, which has to be chosen by experience. Difficulties of the original version of the core-saturation method devised by Kalkofen & Ulmschneider (1984), which were found in extensive acoustic wave calculations by Rammacher & Ulmschneider (1992), can be traced to the frequency discretization and may largely be avoided by a modified core-saturation method. Although these improvements (described in detail below) lead to a more reliable behavior in our wave calculations, we find that the core-saturation method often gives line source functions which are too large, resulting in overestimated line intensities.

Using a large number of iterations with practically infinite core-wing separation parameter $\Delta\tau_\gamma$, the correct line source function can be computed with the core-saturation method. However, in this case the core-saturation method becomes the classical Λ-iteration with its extremely slow convergence rate. The considerable discrepancy of the correct source function as compared to the source function obtained by the core-saturation method demonstrated the weakness of the latter method which could not be improved by a more favorable choice of $\Delta\tau_\gamma$ without increasing the number of iterations (and, correspondingly, the CPU time) to large values.

For these reasons we consider operator splitting methods to obtain more accurate results without increasing the number of iterations or the CPU time for the solution of line transfer problems. This methods are also known as *accelerated Λ-iteration* (ALI) methods (e.g. Olson et al. 1986) or as *operator perturbation* (OP) methods (Kalkofen 1987). However, for the sake of consistency, we will use the term "operator splitting" method (OS) throughout this paper.

Yet, all standard operator splitting methods which we consulted (e.g., MULTI [Carlsson 1986], up to the 1992 version, Kalkofen 1990, private communication) have difficulties in treating media with *discontinuous* changes of physical variables, e.g., stellar atmospheres traversed by shocks. To overcome these problems, we developed an OS method, explicitly accounting for shock discontinuities, which we describe in this paper. Our method, obtained by modifying the approach of Olson & Kunasz (1987), is not only robust, but also very accurate and, moreover, even faster in terms of CPU time than the core-saturation method.

In Section 2, we describe our OS method in detail and give the equations and assumptions used here. This section also describes the modified core-saturation method used by Rammacher & Ulmschneider (1992). Section 3 gives a comparison of the OS method with the modified core-saturation and Λ-iteration methods. Section 4 presents our conclusions.

2. Method

2.1. Radiative transfer in the observers frame

Consider a plane parallel atmosphere traversed by a vertically propagating acoustic wave which causes temperature, T, density, ρ, and velocity, u, fluctuations. The equation of radiative transfer (e.g., Mihalas 1978 p. 449) is then given by

$$\mu \frac{\partial I_{\nu\mu}(z)}{\partial z} = \eta_{\nu\mu}(z) - \chi_{\nu\mu}(z) I_{\nu\mu}(z). \tag{1}$$

Here z is the geometrical height, $I_{\nu\mu}$ the specific monochromatic intensity of the radiation field, μ the angle cosine between the direction of the photons and the outward normal and ν the frequency. The total emissivity is given by $\eta_{\nu\mu}$ whereas $\chi_{\nu\mu}$ describes the total extinction. We consider here the case of a two level atom with background radiation in LTE. The line emission and absorption profiles are calculated assuming complete redistribution (CRD). Then the emissivity and the extinction coefficient can be written as

$$\eta_{\nu\mu}(z) = \eta_{\mathrm{C}}(z) + \eta_{\mathrm{L}}(z)\varphi_{\nu\mu}(z) \tag{2}$$

and

$$\chi_{\nu\mu}(z) = \chi_{\mathrm{C}}(z) + \chi_{\mathrm{L}}(z)\varphi_{\nu\mu}(z), \tag{3}$$

respectively. Here, χ_{L} and χ_{C} are frequency-independent line and continuum extinction, η_{L} and η_{C} are the line and continuum emissivities and $\varphi_{\nu\mu}$ is the absorption profile, given by the Voigt function

$$\varphi_{\nu\mu} = \frac{H(a,v)}{\sqrt{\pi}\Delta\nu_{\mathrm{D}}}, \tag{4}$$

where

$$a = \frac{\Gamma}{4\pi\Delta\nu_{\mathrm{D}}}, \tag{5}$$

$$v = \frac{\nu - \nu_0\left(1 - \mu\, u(z)/c_{\mathrm{L}}\right)}{\Delta\nu_{\mathrm{D}}}, \tag{6}$$

with the damping constant Γ, the thermal Doppler width $\Delta\nu_D$, the gas velocity u, and the speed of light c_L. The absorption profile satisfies the normalization condition

$$\int_{-1}^{1}\int_{-\infty}^{\infty} \varphi_{\nu\mu}\mathrm{d}\nu\mathrm{d}\mu = 1. \tag{7}$$

The background source function is defined as

$$S_{\mathrm{C}} = \frac{\eta_{\mathrm{C}}}{\chi_{\mathrm{C}}} \tag{8}$$

and similarly the line source function as

$$S_{\mathrm{L}} = \frac{\eta_{\mathrm{L}}}{\chi_{\mathrm{L}}}\ . \tag{9}$$

The line source function S_L for the two-level approximation assuming CRD is given by

$$S_{\mathrm{L}}(z) = [1 - \epsilon(z)]\,\overline{J}(z) + \epsilon(z)B(z), \tag{10}$$

where

$$\epsilon(z) = \frac{\epsilon'(z)}{1 + \epsilon'(z)}$$

and with the photon destruction probability (Mihalas 1978, p. 337)

$$\epsilon'(z) = \frac{n_{\mathrm{e}}(z)\Omega_{21}(z)}{A_{21}}\left(1 - \mathrm{e}^{-h\nu/kT(z)}\right). \tag{11}$$

The line profile averaged mean intensity $\overline{J}(z)$ is given by

$$\overline{J}(z) = \frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}\nu\int_{-1}^{1}\mathrm{d}\mu\,\varphi_{\nu\mu}(z)I_{\nu\mu}(z). \tag{12}$$

If we assume that the background source function is Planckian and constant over the line center, $S_{\mathrm{C}}(z) = B(T(z))$, we can write the total source function, $S_{\nu\mu}(z)$, as

$$S_{\nu\mu}(z) = \frac{\varphi_{\nu\mu}(z)S_{\mathrm{L}}(z) + r(z)B(z)}{\varphi_{\nu\mu}(z) + r(z)}, \tag{13}$$

with the residual strength of the continuum, $r(z)$, given by $r(z) = \chi_{\mathrm{C}}(z)/\chi_{\mathrm{L}}(z)$. Following Mihalas (1978) we define

$$\xi_{\nu\mu}(z) = \frac{\epsilon(z)\varphi_{\nu\mu}(z) + r(z)}{\varphi_{\nu\mu}(z) + r(z)} \tag{14}$$

and rewrite Eq. (13) as

$$S_{\nu\mu}(z) = (1 - \xi_{\nu\mu}(z))\overline{J}(z) + \xi_{\nu\mu}(z)B(z), \tag{15}$$

which has the same form as Eq. (10).

Introducing the optical depth along a ray, specified by $(\nu\mu)$,

$$\tau_{\nu\mu}(z) = \frac{1}{\mu}\int_{z}^{z_{\max}}\chi_{\nu\mu}(z)\mathrm{d}z \tag{16}$$

we can write the transfer equation for one ray as

$$\frac{\partial I_{\nu\mu}(z)}{\partial\tau_{\nu\mu}(z)} = \left[I_{\nu\mu}(z) - S_{\nu\mu}(z)\right]. \tag{17}$$

For a given source function $S_{\nu\mu}$, Eq. (17) is readily integrated to obtain the specific intensities for each angle, frequency and depth point. A formal solution, i.e., the calculation of $\overline{J}$ for a known source function, is then completed by using Eq. (12).

2.2. The operator splitting method

Formally, we write the sequence of operations needed to compute $\overline{J}$ for a given source function as

$$\overline{J} = \Lambda[S], \tag{18}$$

the so-called Λ-operation. The operator acting on the source function to obtain $\overline{J}$, is called "Λ-operator". Combining Eqs. (18) and (15) we find

$$S_{\nu\mu}(z) = (1 - \xi_{\nu\mu}(z))\Lambda[S_{\nu\mu}] + \xi_{\nu\mu}(z)B(z). \tag{19}$$

The problem is to solve Eq. (19) for a given model atmosphere with prescribed boundary conditions for the specific intensities (in the following we drop the subscripts to simplify the notation).

The ordinary Λ-iteration proceeds by calculating the (n+1)-th iterate of the source function, S^{n+1}, from the n-th by means of the expression

$$S^{n+1} = (1-\xi)\Lambda[S^n] + \xi B. \tag{20}$$

The well known drawback of this iteration scheme, i.e., slow convergence, can be avoided by splitting the Λ-operator according to

$$\Lambda = \Lambda^* + (\Lambda - \Lambda^*), \tag{21}$$

with an appropriately chosen "approximate Λ-operator", Λ^*. Using Eq. (21), the iteration scheme for the operator splitting then reads

$$S^{n+1} = (1-\xi)\Lambda^*[S^{n+1}] + (1-\xi)(\Lambda - \Lambda^*)[S^n] + \xi B, \tag{22}$$

or, with the formal solution of the n-th iterate, $\overline{J}^{\mathrm{FS}} = \Lambda[S^n]$ and $S^{\mathrm{FS}} = (1-\xi)\overline{J}^{\mathrm{FS}} + \xi B$,

$$\begin{aligned} S^{n+1} - S^n &= \left[1 - (1-\xi)\Lambda^*\right]^{-1}\left[S^{\mathrm{FS}} - S^n\right] \\ &\equiv \mathbf{A}^{-1}\left[S^{\mathrm{FS}} - S^n\right]. \end{aligned} \tag{23}$$

Equation (23) shows that, for robust convergence, Λ^* should contain the essential physics of the line transfer problem and, in order to conserve computer time, should be easy to compute and to invert.

Starting with a first guess for the source function, S^0, the transfer equation Eq. (17) is integrated to compute a formal solution using Eqs. (12) and (15). We then solve Eq. (23) *directly* and obtain an improved value for S. This new source function is subsequently used to calculate a new formal solution. Λ^* and $\mathbf{A}^{-1}$† can be precomputed and reused, thus greatly reducing the number of operations required for a full iteration step. Note that the frequency and angle dependence of the total source function $S_{\nu\mu}$ enters the problem only via $\xi_{\nu\mu}$, Eq.(15). Therefore, we can solve for the frequency independent line source function,

$$S_{\mathrm{L}}^{n+1} - S_{\mathrm{L}}^n = \left[1 - (1-\epsilon)\Lambda^*\right]^{-1}\left[S_{\mathrm{L}}^{\mathrm{FS}} - S_{\mathrm{L}}^n\right]. \tag{24}$$

instead of Eq. (23). The formal solution for the line source function is given by

$$S_{\mathrm{L}}^{\mathrm{FS}} = (1-\epsilon)\overline{J}^{\mathrm{FS}} + \epsilon B$$

where $\overline{J}^{\mathrm{FS}}$ is obtained from the total source function, Eq. (13), as

$$\overline{J}^{\mathrm{FS}} = \Lambda[S_{\nu\mu}^n]. \tag{25}$$

† it is preferable to use LU decomposition for the solution of Eq. (23)

2.3. Formal solution

We consider an atmospheric slab with D grid-points. The depth dependent variables are then vectors with values at the grid-points as components. We use N discrete frequency points $\nu_n, n = 1, \ldots, N$ in the range $-\infty, \ldots, \infty$, covering the width of the line and M discrete angle points $\mu_m, m = 1, \ldots, M$ in the range $\mu = 0, \ldots, 1$. We put the frequency and angle points together in rays labelled by (ν_n, μ_m) and define a ray index as $r = m + (n-1)M$. In this case, the discrete representation of the Λ-operator is a D×D-matrix, and Eq. (18) becomes

$$\overline{J}_d = \sum_{d'} \Lambda_{dd'} S_{d'} \ . \tag{26}$$

The elements of the k-th column, Λ_{dk}, of the exact Λ-matrix are the elements $\overline{J}_d$ of a formal solution obtained using a "pulse" like source function,

$$S_k = 1 \ , S_{d\neq k} = 0 \ , \tag{27}$$

see also Olson et al. (1986).

We treat shocks as discontinuities in the physical variables so that we have to deal with large differences in optical distances $\Delta\tau$ between adjacent grid-points and, at the shock-points themselves with vanishing optical distances, $\Delta\tau = 0$. Another complication arises from the fact that density and temperature, as well as velocity, undergo rapid variations from pre-shock to post-shock regions, causing discontinous jumps in the extinction and the emissivity as well as in $\overline{J}$. On the other hand, the monochromatic specific and mean intensities are continuous over the shock-points, which must be reproduced by the numerical solution. Therefore, to compute the formal solution, we integrate the transfer equation using a piecewise linear interpolation to the source function. For such an interpolation, Kalkofen & Ulmschneider (1984) showed that the specific intensities along an outgoing ray can be written as

$$I_{dr}^+ = a_{dr}^+ I_{(d+1)r}^+ + b_{dr}^+ S_{dr} + c_{dr}^+ S_{(d+1)r} \ , \tag{28}$$

with

$$\begin{aligned} a_{dr}^+ &= \frac{2-\delta}{2+\delta}; \quad b_{dr}^+ = c_{dr}^+ = \frac{\delta}{2+\delta}, \quad \delta \leq 1 \\ a_{dr}^+ &= c_{dr}^+ = \frac{1}{2\delta+1}; \ b_{dr}^+ = \frac{2\delta-1}{2\delta+1}, \quad \delta > 1 \end{aligned} \ , \tag{29}$$

where

$$\delta = \tau_{(d+1)r} - \tau_{dr}. \tag{30}$$

Here τ_{dr} denotes the optical depth at grid-point d along the outgoing ray with index r. The superscript "+" denotes outgoing ($\mu > 0$) radiation. Similarly we find for the ingoing ($\mu < 0$, superscript "−") intensities

$$I_{dr}^- = a_{dr}^- I_{(d-1)r}^- + b_{dr}^- S_{dr} + c_{dr}^- S_{(d-1)r} \ , \tag{31}$$

where the values a_{dr}^-, b_{dr}^-, c_{dr}^- are the same as the a_{dr}^+, b_{dr}^+, c_{dr}^+ except that now

$$\delta = \tau_{dr} - \tau_{(d-1)r} \ , \tag{32}$$

with the optical depth along the ingoing ray. The formal solution is then obtained by integrating the specific intensities over all rays and directions as indicated by Eq. (12).

2.4. Choice of Λ^*

As indicated above, the elements of the exact Λ-matrix can be obtained by applying Eqs. (28) and (31) to the unit "pulse" source function.

Olson et al. (1986, OAB) showed, that a good choice for Λ^* is the main diagonal of the exact matrix. In that case, Λ^* is a diagonal matrix and their method is the classical Jacobi-method for the solution of linear equations. Using a tri-diagonal Λ^*, Olson & Kunasz (1987, OK) could improve the convergence rate considerably and decrease the amount of CPU time required for the solution of line transfer problems. In addition, they introduced the so-called *short-characteristics method* to calculate the formal solution for the specific intensities. Our approach to the solution of the transfer equation (17), using Eqs. (28)-(32) closely resembles the method used by OK, with the main advantage that the costly calculations of exponentials are avoided. Furthermore, our choice of quadrature coefficients, Eq. (29), *unconditionally guarantees* a stable solution of the transfer equation, even for the very irregular τ-grids encountered in our hydrodynamic calculations (Kalkofen & Wehrse 1982). In addition, this form of the formal solution gives the correct run of the intensity over the shock points.

In our hydrodynamical wave calculations, we use the tridiagonal Λ^* with Ng-Acceleration (Auer 1987, 1991). The speed of the method is further improved by using the source function S from the old hydrodynamic time step as starting value for the operator splitting in the following time step. For temperature-correction methods used to obtain an initial model atmosphere, we found that the best choice is a Λ^* with a bandwidth of nine for calculations performed on an IBM 3090-180VF (see Hauschildt [in preparation] for a discussion on the performance of the ALI method as a function of the Λ^* bandwidth).

2.5. The modified core-saturation method

Since the modified core-saturation method used by Rammacher & Ulmschneider (1992) has not yet been described in detail, we briefly outline it here. In the original core-saturation method the source function, S_L, in Eq. (10) (see Kalkofen & Ulmschneider 1984) can be written

$$S_L = \frac{\frac{1}{2}\int_{\text{wing}}\int \varphi_{\nu\mu}\, I_{\nu\mu}\, d\nu\, d\mu + \epsilon' B}{p_e + \epsilon'} = \frac{J_{\text{wing}} + \epsilon' B}{p_e + \epsilon'}, \tag{33}$$

where p_e is the escape probability, given by

$$p_e \equiv \frac{1}{2}\int_{\text{wing}}\int \varphi_{\nu\mu}\, d\nu\, d\mu \quad . \tag{34}$$

The crucial point of the core-saturation method is the core-wing separation. The integrals in Eqs. (33) and (34) are taken only over the line wings. Which frequencies belong to the line core and which to the line wings depends on the optical depth and the physical state (velocity, temperature, etc.) of the atmosphere. For a given frequency point, ν_n, the source function, S_L, at depth τ_d belongs to the line wing if

$$\Delta\tau_{dnm} = \tau_{dnm} - \tau_{(d-1)nm} \leq \Delta\tau_\gamma, \tag{35}$$

and to the line core otherwise. $\Delta\tau_\gamma$ is a free, but fixed, parameter, usually taken equal to unity. If shocks are present, the shock points can approach regular grid-points arbitrarily close. In those cases the criterion Eq. (35) must be scaled in comparison to the optical distance between adjacent regular grid-points (see Kalkofen & Ulmschneider 1984). As a practical convergence criterion used in the core-saturation method we use, typically, the relative change of the source function in each iteration. Note that this criterion is useful *only* if the convergence rate of the method is sufficiently fast. Otherwise the well-known problems with this simple criterion in the case of the Λ-iteration would also apply to the core-saturation method. Therefore, in order to be useful in our calculations, the core-saturation method must converge with a rate comparable to that of the operator splitting method. In the following discussion, we assume that the relative change of the source function versus iteration number is used as a convergence criterion (hereafter,"standard criterion"), typically we require that the source function does not change by more than 0.1 % in subsequent iterations.

When this core-saturation method was used to compute a time-sequence of spectral line features (e.g. the emission peaks of the Ca II K line) during acoustic wave calculations (Rammacher & Ulmschneider 1992, Fig. 5) we found that strong oscillations in intensity were superposed over the regular time development of the line intensity. This is clearly caused by a too slow convergence rate of the core-saturation method, resulting in relatively large errors in the source function if the standard convergence criterion was used. We discovered that this was due to the crudeness of the criterion Eq. (35) which in one particular situation might be easily satisfied, while in another just barely so. As the largest contributions to the wing integrals occur at the innermost frequencies just adjacent to the core-wing separation, this crudeness of the criterion translated itself into considerable intensity variations from one time step to the next.

That this explanation indeed was the source of the unphysical intensity oscillations could be demonstrated by computing wing contributions at additional frequency points (two frequencies ν_j, ν_k on each side of the line for every depth point d) such that Eq. (35) was always satisfied with an equal sign ($\Delta\tau_{djm} = \Delta\tau_{dkm} = \Delta\tau_\gamma$). Note that these frequencies can easily be found by interpolation between neighboring frequencies at the core-wing boundary (e.g. $\Delta\tau_{dnm} < \Delta\tau_\gamma$ and $\Delta\tau_{d(n+1)m} > \Delta\tau_\gamma$). This procedure greatly improved the results of the core-saturation method, but because of the additional 2N frequency points, made it too slow for our time-dependent computations.

After some experimentation we found the following compromise between convergence rate and speed which we subsequently used in the calculations of Rammacher & Ulmschneider

(1992). With the frequencies ν_j, ν_k found as described above for every grid-point d we compute at this depth point a modified escape probability

$$p_{e'} \equiv \frac{1}{2}\left(\int_{\nu_1}^{\nu_j}\int \varphi_\nu \, d\nu d\mu + \int_{\nu_k}^{\nu_N}\int \varphi_\nu \, d\nu d\mu\right), \quad (36)$$

from which we obtain a correction factor $f_{\rm corr}$

$$f_{\rm corr} \equiv \frac{p_e}{p_{e'}}. \quad (37)$$

The wing integral can then be estimated by

$$J'_{\rm wing} = \frac{J_{\rm wing}}{f_{\rm corr}}. \quad (38)$$

Here p_e and $J_{\rm wing}$ are calculated using only the regular frequency grid. This modified core-saturation method, where we replace p_e and $J_{\rm wing}$ in Eq. (33) by the values $p_{e'}$ and $J'_{\rm wing}$, requires only a small amount of additional numerical work when compared to the standard core-saturation method. Note that $f_{\rm corr}$ does not enter the iteration process for $J'_{\rm wing}$ and thus an error does not get amplified, ensuring the stability of the scheme.

3. Comparison of the methods

3.1. The operator splitting method

As a typical application we consider here an acoustic wave calculation in a plane parallel stellar atmosphere. In these calculations, we will normally find a few shocks travelling through the atmosphere at any given time. The shocks eventually reach the line forming region, where in the transfer calculation they must be treated accurately in order to obtain realistic line profiles and line cooling rates. As an instructive example, we show in Fig. 1 a monochromatic acoustic wave in the solar atmosphere (Rammacher & Ulmschneider 1992, Figs. 1&2).

A good example is the time-dependent line transfer problem for the Ca II K line. The K line is strongly dominated by scattering and an important diagnostic tool for analyses of solar and stellar chromospheres and coronae. We use 29 logarithmically spaced frequency points up to ± 10Å from line center and one angle point $\pm|\mu|$ in a two stream approximation. For simplicity, we assume complete redistribution, although more realistic calculations will have to include effects of partial redistribution. For the atomic data used see Rammacher & Ulmschneider (1992) as well as Kalkofen et al. (1984).

Using the methods discussed above, numerically identical solutions can be obtained because for all methods we use identical grids and formal solution procedures. To simplify the discussion of the results, we use in the following discussion the symbol '∞' to denote solutions which have converged to machine accuracy (approximately 10^{-15} for the machines used here). If $E(d) = |S(d) - S(d)_\infty|/S(d)_\infty$ denotes the relative error of the source function at a (geometrical) grid-point d for a given iteration number, then the maximum error can be defined as EMAX = max($E(d)$). Figure 2 shows the maximum error

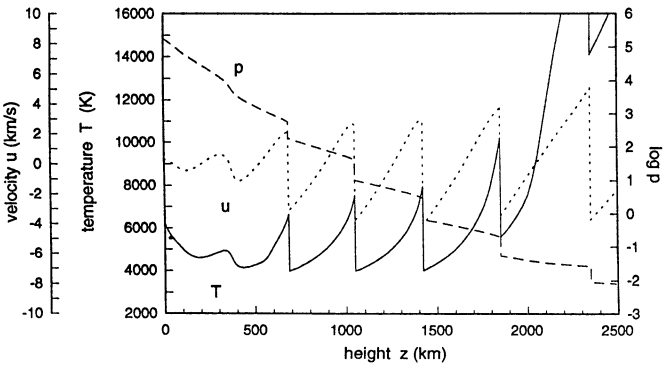

Fig. 1. Acoustic wave with period $P = 45\ s$ and initial energy flux $F_M = 2 \cdot 10^8\ erg\ cm^{-2}\ s^{-1}$ after Rammacher & Ulmschneider (1992). Temperature T (K), velocity u (km/s), pressure $log\ p$ (dyn/cm^2) are shown as function of the Eulerian height z (km)

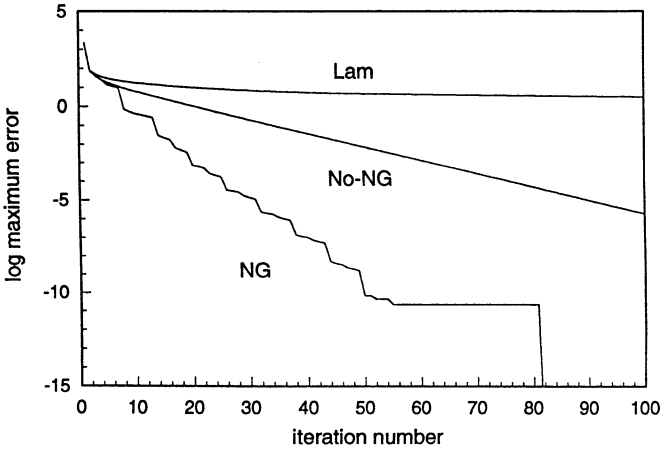

Fig. 2. Maximum error EMAX versus iteration number for different methods. The operator splitting method of this paper with Ng-acceleration is labeled *Ng*, without Ng-acceleration *non-NG* and for the Λ-iteration *Lam*

as function of the iteration number for the Λ-iteration, the OS method, and the OS method in combination with the Ng convergence acceleration (Auer 1987, 1991). The iterations start with $S(z) = B(T_e(z))$, where $T_e(z)$ is the electron temperature at the depth z.

For the OS method combined with the Ng-acceleration we find that the source function has converged to machine accuracy after about 80 iterations. The convergence rate is very similar to that found by Hauschildt (1992) in the case of Lagrangian frame line transfer in relativistically expanding spherical shells. Convergence is considerably slower if the Ng-acceleration is not used, and it is extremely slow if the Λ-iteration method is used (the Ng-acceleration is not effective with the Λ-iteration, see Auer [1987]). All methods converge, eventually, to machine accuracy, for the OS method without Ng-acceleration after about 180 and in the case of the Λ-iteration after about 90000 iterations. The convergence of the Λ-iteration is shown in Fig. 3. In all three cases the identical '∞' solution is finally reached.

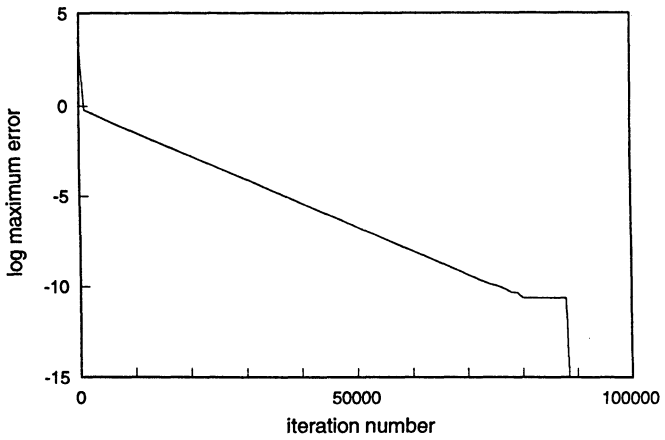

Fig. 3. Maximum error EMAX versus iteration number for a large number of iterations in the case of the Λ-iteration

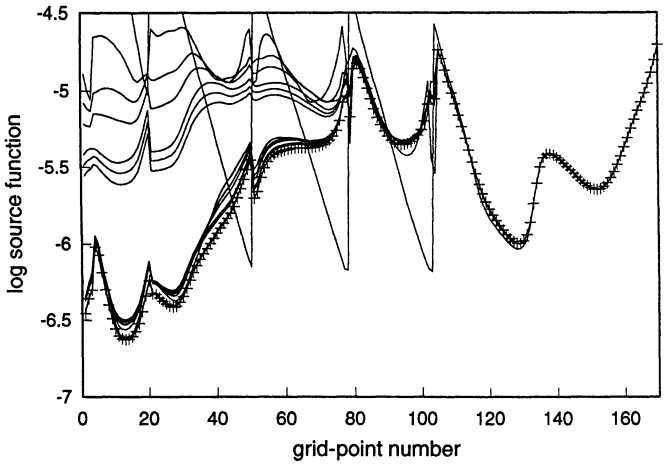

Fig. 4. Source function versus grid-point number, counted inwards from the top of the atmosphere, for the first 18 iterations. The final solution (machine accuracy after 100 iterations) is shown also and indicated at the grid-points by + signs

From the above results it is obvious that a reasonable accuracy of EMAX = 0.1% is attained after about 20 ALI iterations if Ng-acceleration is used. The run of the source functions versus grid-point number, for the first 18 iterations are shown in Fig. 4. The converged solution of the line source function is marked by '+' symbols. In Fig. 4 grid-point numbers are used as abscissa as here the infinitesimally close pre-shock and post-shock points can be plotted more clearly. The geometrical distance between two grid-points, except near the shock points, is about 15 km and we have used a total of 170 non-shock height points, with 2 additional points per shock.

The discontinous run of $T_e(z)$ at the shock points is clearly seen in the initial guess of the source function. The non-local effects of radiation transport quickly smooth most of the discontinuities of the line source function. However, due to the non-negligible coupling of the source function to the thermal electrons via the collisional rates, smaller discontinuities in the source function remain. Due to the shifting and broadening of the line profile caused by the temperature and velocity jumps across the shock front, the source function at the hot and dense post-shock region happens to be *smaller* than at the pre-shock region. The behavior of the iteration process and the convergence rate in our case is similar to that found by Auer (1987, 1991) and Hauschildt (1992).

3.2. *The modified core-saturation method*

The basic idea of the core-saturation method is to treat the radiation transport only in the optically thin line wings. Thus the convergence rate depends on the core-wing separation, that is, on the choice of $\Delta\tau_\gamma$. The idea is, that for a small value of $\Delta\tau_\gamma$ the Λ-iteration, which is used in the optically thin wings only, can be brought to rapid convergence and thus the large number of iterations necessary for a pure Λ- iteration can be avoided. In principle, for an ideal method, the final results for the source function *must* be independent of the choice of $\Delta\tau_\gamma$, even if the simple standard convergence criterion is used. Figure 5 shows the rapid approach to a 'converged' source function of the modified core-saturation method for the choice $\Delta\tau_\gamma = 1$

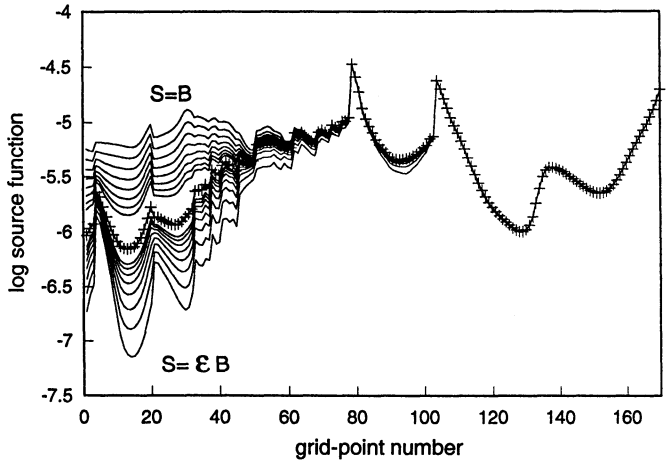

Fig. 5. Source function versus grid-point number for the modified core-saturation method and $\Delta\tau_\gamma = 1$ starting from $S = B$ (upper curves) or from $S = \epsilon B$ (lower curves). Iteration numbers 5 to 12 are shown together with the converged source function indicated by + signs

used extensively by Rammacher & Ulmschneider (1992). The upper curves show the results obtained by using $S = B$ as initial guess of the line source function, whereas the lower curves show the results for $S = \epsilon B$ as initial guess. In Fig. 5 only iteration numbers 5 to 12 are shown and the 'converged' source function is indicated by the + symbols. The 'converged' source function is here defined by requiring that the maximum relative change of S in two subsequent iteration is less than 0.1 %, which corresponds in this particular case to about 20 iterations.

Unfortunately, as shown in Fig. 6, this source function shows distinctive differences compared to the truly converged source function S_∞. At the top of the atmosphere the core-saturation method in combination with the standard convergence criterion leads to a considerable overestimate of the source function which could be improved by selecting higher values of $\Delta\tau_\gamma$.

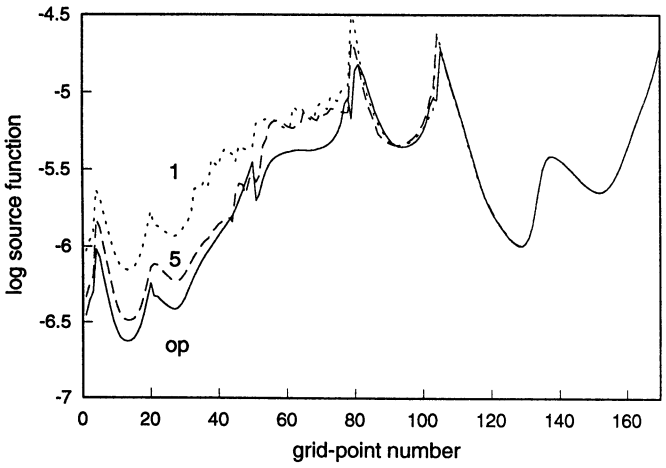

Fig. 6. Converged source functions versus grid-point number using the modified core-saturation method with parameters $\Delta\tau_\gamma = 1$ (labeled 1) and $\Delta\tau_\gamma = 5$ (labeled 5), together with the final solution obtained from our present operator splitting method (labeled *op*)

Figure 6 shows the source function obtained using $\Delta\tau_\gamma = 5$. However, to satisfy the standard convergence criterion for this value of the core-wing separation about 80 iterations are necessary for that same termination condition. With increasing $\Delta\tau_\gamma$ the number of necessary iterations rapidly increases as we approach the case of a pure Λ-iteration. Here then the advantage of the core-saturation method as a fast method is lost. This could be improved if we use Ng-acceleration also for the core-saturation method.

However, even for $\Delta\tau_\gamma = 5$ we find considerable differences compared to the truly converged source function S_∞. The overestimate of the source function in the middle to high chromosphere and particularly behind the shocks is only partly reduced. From this we conclude that the core-saturation method, independent of the choice of $\Delta\tau_\gamma$, is much less accurate than the operator splitting method. In addition, in terms of computational speed the OS method is faster than the core-saturation method with $\Delta\tau_\gamma = 1$ because of its faster convergence rate.

4. Conclusions

We have developed a fast, robust and accurate operator splitting method for the solution of spectral line radiative transfer problems assuming complete redistribution. Our method allows to simulate stellar atmospheres with shock discontinuities in time-dependent calculations. This method is much more accurate and even superior in speed, in particular if Ng-acceleration is used, than the modified core-saturation method and does not depend awkwardly on a parameter like $\Delta\tau_\gamma$. It is easy to implement and very reliable. This is accomplished by using a tri-diagonal approximate Λ^*-operator which results in an enormous increase in the convergence rate of the OS iteration when compared to the Λ-iteration or even the OS method using a diagonal Λ^*-operator.

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Appendix

As indicated in Chap. 2 we solve the discretized transfer equation, Eqs. (28)-(31) for a pulse like source function $S_k = 1$, $S_{j\neq k} = 0$. The resulting specific intensities are integrated over frequency and angle using Eq. (12), to obtain the formal solution $\overline{J}$. The elements of $\overline{J}$ are the elements of the k-th column of the Λ-matrix. The frequency quadrature is performed with a trapezoidal rule whereas the angle integration uses Gaussian quadrature scheme. We combine the appropriate quadrature weights

$$w_r = w_n w_m \ , \ r = 1, \ldots, R = NM$$

to obtain the integration weights for one ray, w_r. We thus have for the first column:

$$\Lambda_{11} = \frac{1}{2}\sum_{r=1}^{R} w_{1r}\varphi^+_{1r}b^+_{1r}$$

$$\Lambda_{21} = \frac{1}{2}\sum_{r=1}^{R} w_{2r}\varphi^-_{2r}c^-_{2r}$$

$$\Lambda_{(l\geq 3)1} = \frac{1}{2}\sum_{r=1}^{R} w_{lr}\varphi^-_{lr}\cdot\left(\left(\prod_{j=3}^{l} a^-_{jr}\right)c^-_{2r}\right) \ , \qquad (1)$$

for the k-th column:

$$\Lambda_{(l\leq k-2)k} = \frac{1}{2}\sum_{r=1}^{R} w_{lr}\varphi^+_{lr}\left(\left(\prod_{j=l}^{k-2} a^+_{jr}\right)\right.$$
$$\left.\times(a^+_{(k-1)r}b^+_{kr} + c^+_{(k-1)r})\right)$$

$$\Lambda_{(k-1)k} = \frac{1}{2}\sum_{r=1}^{R} w_{(k-1)r}\varphi^+_{(k-1)r}$$
$$\times(a^+_{(k-1)r}b^+_{kr} + c^+_{(k-1)r})$$

$$\Lambda_{kk} = \frac{1}{2}\sum_{r=1}^{R}(\varphi^+_{kr}b^+_{kr} + \varphi^-_{kr}b^-_{kr})$$

$$\Lambda_{(k+1)k} = \frac{1}{2}\sum_{r=1}^{R} w_{(k+1)r}\varphi^-_{(k+1)r}$$
$$\times(a^-_{(k+1)r}b^-_{kr} + c^-_{(k+1)r})$$

$$\Lambda_{(l\geq k+2)k} = \frac{1}{2}\sum_{r=1}^{R} w_{lr}\varphi^-_{lr}$$
$$\times\left(\left(\prod_{j=k+2}^{l} a^-_{jr}\right)(a^-_{(k+1)r}b^-_{kr} + c^-_{(k+1)r})\right) \qquad (2)$$

and for the D-th column:

$$\Lambda_{(l\le D-1)D} = \frac{1}{2}\sum_{r=1}^{R} w_{lr}\varphi^{+}_{lr} \times \left(\left(\prod_{j=l}^{D-2} a^{+}_{jr}\right) c^{+}_{(D-1)r}\right)$$

$$\Lambda_{(D-1)D} = \frac{1}{2}\sum_{r=1}^{R} w_{(D-1)r}\varphi^{+}_{(D-1)r} c^{+}_{(D-1)r}$$

$$\Lambda_{DD} = \frac{1}{2}\sum_{r=1}^{R} w_{Dr}\varphi^{-}_{Dr} b^{-}_{Dr} \,. \qquad (3)$$

Again, the superscripts"+" and "−" denote the coefficients and profile functions of outgoing and ingoing rays, respectively.

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