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The use of iteration factors in the solution of the NLTE line transfer problem—II. Multilevel atom

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ABSTRACT

The iteration factors method (IFM) developed in Paper I [1] (Atanacković-Vukmanović and Simonneau, 1994) to solve the NLTE line transfer problem for a two-level atom model, is extended here to deal with a multilevel atom case. At the beginning of each iteration step, for each line transition, angle and frequency averaged depth-dependent iteration factors are computed from the formal solution of radiative transfer (RT) equation and used to close the system of the RT equation moments, non-linearly coupled with the statistical equilibrium (SE) equations. Non-linear coupling of the atomic level populations and the corresponding line radiation field intensities is tackled in two ways. One is based on the linearization of the equations with respect to the relevant variables, and the other on the use of the old (known from the previous iteration) level populations in the line-opacity-like terms of the SE equations. In both cases the use of quasi-invariant iteration factors provided very fast and accurate solution. The properties of the proposed procedures are investigated in detail by applying them to the solution of the prototype multilevel RT problem of Avrett and Loeser [2], and compared with the properties of some other methods.

1. Introduction

NLTE radiative transfer (RT) problems are among the most difficult ones to deal with due to the important role of scattering process which makes the properties of very distant points in a medium non-locally coupled through the radiation field. The multilevel line transfer problem is especially difficult as it is in addition non-linear; the atomic level populations and the radiation field intensities in the corresponding line transitions are non-linearly coupled via the statistical equilibrium (SE) equations. Therefore, the problem requires a simultaneous solution of the RT and SE equations, which can be achieved only through an iterative method. The various methods basically differ in the way that linearity is achieved at each iterative step, with *linearization* and *preconditioning* being the two most used mathematical strategies [3].

The first self-consistent solutions of the RT problems were obtained by the complete linearization (CL) method, developed originally for the stellar atmosphere modelling by Auer and Mihalas [4], and later applied to the NLTE line formation problem by Auer [5]. It consists in the linearization of all coupled equations by expansion to the first order of the relevant variables around an initial estimate and in the simultaneous determination of the variables' increments (corrections). The convergence rate of this global approach is high. However, for a good description of the physical system a very large number of frequency, angle and depth points is usually needed, involving big matrices and requiring huge memory storage and a lot of computing time.

Therefore, more simple and efficient iterative methods were developed. Such methods use a sequential iterative

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procedure, taking advantage of the fact that a problem can be divided into separate tasks according to the physics of the problem and the mathematical properties of the relevant equations (see, e.g., the overviews [6,7]). The current solution of each individual task is obtained by assuming that the output of the others is known. Thus each task can be optimized independently. More specifically, in the multilevel line formation problem, each step of the iterative procedure is usually split into two parts so that within each of them, one of the two systems of equations, RT and SE, is solved by taking the solution, or part of the solution, of the other one as known. The coupling is performed at the end of the iterative procedure, with the convergence rate that depends on the amount of information transferred between the two parts.

The simplest sequential iterative procedure, the so-called Λ iteration, solves the problem equations alternately. Although conceptually completely different, the CL method and the Λ iteration method are akin in the sense that both use the exact description of the RT process (the full lambda operator). However, the convergence of this simplest iterative scheme is in most cases of interest extremely slow, as it transfers from one part of the iterative step to the other more information than necessary.

Several classes of iterative methods for NLTE line transfer problems, converging rapidly towards the exact solution, have been developed so far.

One of the first attempts to facilitate the solution of multilevel line transfer problem was the so-called ETLA (equivalent-two-level-atom) approach developed by Avrett [8] and described by Mihalas [9] and Avrett and Loeser [2]. It simplifies the use of the SE equations so that only one transition in the model atom at a time is combined with the transfer problem and the coupling of all levels is achieved by iteration over all transitions.

An other approach employs certain approximation to simplify the detailed description of the RT process, i.e. it uses an approximate lambda operator (ALO) instead of the exact one [10], accounting for a small error introduced by this approximation iteratively [11]. This is the basic idea of a very broad class of the so-called accelerated/approximated lambda iteration (ALI) methods. The approximation is based either on the physics of the transport of photons through the medium (e.g. core saturation assumption of Rybicki [12]) or on some mathematical considerations (e.g. the diagonal of the full Λ operator is proposed as an ALO by Olson et al. [13]). To achieve the linearity at each iterative step ALI methods usually employ either linearization (e.g. Scharmer and Carlsson [14]) or preconditioning (e.g. Rybicki [12], Rybicki and Hummer [15]) of the equations. A brief review of ALI methods was already given in Paper I (for more details see also Rybicki [16] and more recent reviews by Hubeny [6] and Carlsson [17]). Here, we shall mention only the methods, the solutions or properties of which will be compared with those obtained by the iteration factors method (IFM), developed in this paper. One is the so-called MALI (multilevel accelerated lambda iteration) method by Rybicki and Hummer [15], who were the first to introduce ALOs directly into the SE equations (preconditioning). The MALI method was successfully applied to the solution of various multilevel RT problems (e.g. in multidimensional multilevel line RT by Auer et al. [18], in isolated solar atmospheric structures by Heinzel [19] or in multilevel RT with partial frequency redistribution by Paletou [20] and Uitenbroek [21]). Other numerical methods for NLTE RT applications that dramatically accelerate the Λ iteration are the Gauss–Seidel (GS) and successive overrelaxation (SOR) methods of Trujillo Bueno and Fabiani Bendicho [22], the generalization of which to the multilevel atom case was suggested in the same paper, and summarized in Section 2 of the paper by Fabiani Bendicho et al. [23]. The implementation details of their multilevel Gauss–Seidel (MUGA) method were made explicit by Asensio Ramos and Trujillo Bueno [24] (see also [25]). Another extremely fast method is the forth-and-back implicit lambda iteration (FBILI) of Atanacković-Vukmanović et al. [26]. The convergence properties of these latter methods compared to those of other ALI methods are discussed in the papers [22–27].

The alternative way to speed up the convergence of the classical Λ iteration is the iteration factors method. The basic idea of this method is in the use of functions—the so-called iteration factors (IFs)—as the inputs/outputs of individual tasks, which, in order to ensure fast and stable iterative procedure, have to be good quasi-invariants along the iterations. At each iteration step the factors are computed from the current solution and then used to update it. Hence, by introducing appropriate modifications in the simple Λ iteration scheme, it is possible to achieve an extremely high convergence rate.

Since the first idea of iteration factors in the radiative transfer literature that appeared in the paper by Feautrier [28], many different applications of the IFs have been discussed [1,20,21,28–38]. Feautrier suggested that the use of the ratio of two moments of the radiation field intensity could speed up the stellar atmosphere model computations. The first realization of the idea was the variable (depth-dependent) Eddington factor (VEF) technique developed for the solution of the monochromatic transfer problem in plane-parallel [29] and in spherical geometry [30]. Auer and Mihalas [29] were the first to iterate on the ratio of two angular moments of the radiation field K_ν/J_ν. They stressed that it is much better to iterate on the ratio of two quantities than on the quantities themselves, as the ratio changes much less from one iteration to another. The VEFs have also been successfully applied to the complete linearization method for both the stellar atmosphere modelling and the line formation problem to reduce the numerical description of the system for its angular dimensions. They enabled a complex explicit frequency-angle coupling to be simplified, so that only the frequency coupling is treated explicitly, whereas the angle coupling is treated iteratively. However, a very large number of frequency points, necessary for a good description of the physical system still made the computations with the CL/VEF (the complete linearization method using VEF) demanding. One could say that the CL/VEF was the predecessor of the so-called hybrid methods which combine the advantages

of its constituents (see e.g. Hubeny [35], Heinzel et al. [36] and Hubeny and Lites [37] for the ETLA/IF/CL method, and Paletou [20], Uitenbroek [21] and Heinzel and Anzer [38] for the MALI/IF method, both of which use the ratio ρ_v of the emission to the absorption profile coefficients as an *iteration factor* in the solution of multilevel line transfer with partial redistribution, or Hubeny and Lanz [39] for the hybrid CL/VEF/ALI method used in stellar atmosphere modelling).

Memory storage and a cost per iteration in the solution of NLTE line transfer problem can be drastically reduced by the use of both angle and frequency averaged iteration factors. Such factors, defined for a line as a whole, were used for the first time in the solution of the linear two-level atom line formation problem in the paper by Atanacković-Vukmanović and Simonneau [1], hereinafter referred to as Paper I. Owing to the use of these factors the exact and fast-convergent solution is achieved with no matrix calculations.

In the present paper we extend the IF method developed in Paper I to the solution of the multilevel line transfer problem. We propose an iterative procedure which overcomes the above-mentioned drawback of the CL/VEF method, retaining its favorable convergence properties while becoming computationally cheap owing to the use of both angle and frequency averaged iteration factors. In the first part of each iteration, for each line transition, the iteration factors are computed as the ratios of the relevant intensity moments obtained from the formal solution of the RT equation. They are then used to close the system of the RT equation moments (for all line transitions) non-linearly coupled with the statistical equilibrium (SE) equations (for all level populations). We use two approaches to solve these two systems of equations simultaneously. The first one is based on the linearization of the equations by neglecting the second- and higher-order terms. A substitution of the linearized SE equations into the linearized RT equation moments yields the system of equations that involve only the corrections of the frequency integrated mean intensity of the radiation field explicitly. In the second approach, we obtain the linear form of the SE equations by assuming that the level populations in their line-opacity-like terms are known from the previous iteration [15,40]. Thus we derive linear relations between each line source function and the full set of the radiation field mean intensities and solve them together with the RT equation moments for all line transitions linearly coupled in this way. On one hand this is rather the method insensitive to the poor conditioning of the original equations than the method which copes with this problem by preconditioning [12]. On the other hand, the use of line opacities from the previous iteration in the SE equations, which enables to derive the linear relationships between each line source function and all the radiation field mean intensities, can be considered as a kind of preconditioning. Therefore, for the sake of simplicity we denote our second approach as "preconditioning". In both approaches an extremely fast convergence is provided by the use of quasi-invariant iteration factors in the linearly coupled RT moment and SE equations.

The aim of the present paper is to generalize the IF method developed in Paper I to the solution of the multilevel line transfer problem, to test its accuracy and convergence properties on some benchmark problem, compare it with some of the existing methods used to solve the same kind of the RT problems, and assess its advantages and limitations. Thus, the outline of this paper is as follows. In Section 2 we formulate the multilevel line formation problem, limiting ourselves to the complete redistribution pure line transfer problem in a constant property medium, and leaving the application of the IF method to more realistic calculations for the forthcoming paper (Paper III). In Section 3 we describe the Iteration Factors Method proposed to solve this problem using two families of iteration factors, defined in Paper I, and two ways to solve the non-linear coupling of the RT and SE equations (linearization and "preconditioning"). In order to assess the convergence properties of our method, and to check the accuracy of the solutions against the known ones, in Section 4 we solve the prototype problem by Avrett and Loeser [2] of multilevel line formation (a three-level H atom model) with no background continuum in a plane-parallel constant-property medium and compare its solutions with the existing ones. Finally, in Section 5 we draw our conclusions.

2. Multilevel atom line formation problem

The problem of line radiative transfer in a given atmospheric model consists in the determination of the radiation field and the state of the matter by simultaneous solution of the RT and SE equations. The coupling between the excitation state of the matter and the radiation field intensity is highly non-local as the radiation field at one depth point, via the RT equation, depends on the opacity and emissivity, i.e. on the atomic level populations at all other depth points of the medium. In turn, the level populations depend on the mean intensity of the radiation field via the statistical equilibrium equations.

Compared to the two-level-atom case in which the line source function (i.e. the ratio of emissivity to opacity) can be expressed explicitly as the linear function of the mean line radiation field intensity, with multilevel line transfer there is an additional difficulty due to a strong non-linear coupling among atomic level populations and the corresponding line radiation fields.

Here, we shall limit our discussion to a time independent, plane-parallel and semi-infinite atmosphere of constant physical properties. Assuming complete redistribution (CR), the radiative transfer equation for any line transition ij between two discrete energy levels i and j ($E_j > E_i$) with no background continuum has a dimensionless form:

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

where we dropped indices ij for simplicity; $I_{x\mu}$ is the specific intensity of the radiation field at the mean line optical depth τ, x is the frequency displacement from the line center in Doppler-width units $\Delta\nu_D$, and μ is the cosine of the angle between the direction of photon propagation

and the outward normal. The quantity φ_x is the absorption-line profile, normalized to unity. Under the assumption of complete redistribution the line source function S is frequency independent. Then, for each transition ij, the line source function depends only on the ratio of the corresponding level populations n_i and n_j:

$$S^{ij} = \frac{n_j A_{ji}}{n_i B_{ij} - n_j B_{ji}} = \frac{2hv_{ij}^3}{c^2} \frac{1}{\frac{n_i}{n_j}\frac{g_j}{g_i} - 1}. \quad (2)$$

In the above expression A_{ji}, B_{ij} and B_{ji} are Einstein coefficients of the relevant radiative transitions, while g_i and g_j are statistical weights of the atomic levels. This is the implicit expression for the line source function as the level populations depend on the radiation field intensity through the statistical equilibrium equations (or rate equations). At each depth point for each atomic level j of an NL-level atom we have an equation of the form (e.g. Mihalas [9]):

$$n_j \left\{ \sum_{i<j} (A_{ji} + B_{ji} J_\varphi^{ij} + C_{ji}) + \sum_{k>j} (B_{jk} J_\varphi^{jk} + C_{jk}) \right\} = \sum_{i<j} n_i (B_{ij} J_\varphi^{ij} + C_{ij}) + \sum_{k>j} n_k (A_{kj} + B_{kj} J_\varphi^{jk} + C_{kj}), \quad (3)$$

where C's are the inelastic collisional rates. The atomic level populations depend on the radiation field in different line transitions via the terms that contain the so-called scattering integrals:

$$J_\varphi^{ij}(\tau) = \int_{-\infty}^{\infty} \varphi_x J_x(\tau)\, dx = \int_{-\infty}^{\infty} \varphi_x\, dx \frac{1}{2} \int_{-1}^{1} I_{x\mu}(\tau)\, d\mu, \quad (4)$$

i.e. the frequency averaged mean intensities weighted by the line absorption profile. Finally, for the NL- level atomic model, $NL-1$ linearly independent SE equations are closed by the particle conservation equation:

$$\sum_{i=1}^{NL} n_i = n_{\text{total}}, \quad (5)$$

where n_{total} is the total number density of atoms.

The SE equations (3) can be written formally as

$$\mathbf{P}\overline{n} = \overline{b}, \quad (6)$$

where $\mathbf{P}$ is the rate matrix, $\overline{n}$ is the vector of atomic level populations and $\overline{b}$ is the right-hand side vector. The elements of the rate matrix are, therefore, given by the radiative and collisional rates, except for the last row corresponding to the particle conservation equation.

3. The iteration factors method

While for the linear two-level-atom line formation problem either an iterative or a direct (differential or integral) method can be applied, for the solution of non-linear multilevel problem an iterative procedure is required. To solve this problem, here we propose the iteration factors method, the algorithm of which is given in Fig. 1. Let us briefly describe its main steps.

In the first part of each iteration, starting from a given (e.g. LTE) source function S^o or the one known from the previous iteration step S^i we formally solve the RT Eq. (1)

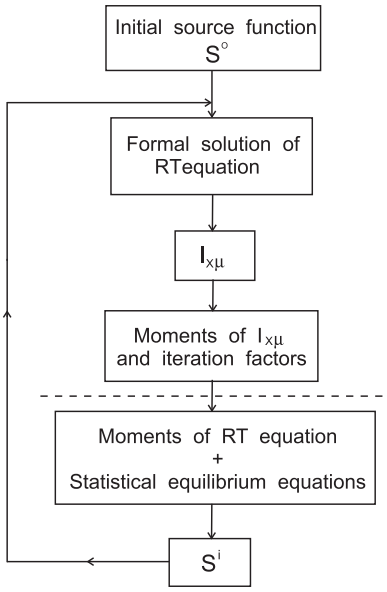

Fig. 1. Flow-chart of the iteration factors method. Horizontal dashed line divides the algorithm into two parts that can be independently optimized (see the text for details).

for each line transition. The numerical solution of the RT equation requires a discrete set of optical depth points τ_d ($d = 1, N$) at which the specific intensities $I_{x\mu}$ for each chosen frequency x_i ($i = 1, NF$) and direction μ_j ($j = 1, ND$) are to be computed. As the radiative transfer is a two-point boundary value problem, we use the two-stream model of the radiation field and compute the inward specific intensities $I^-_{x\mu}(\tau_d)$ starting with the upper boundary condition $I^-_{x\mu}(\tau_1) = 0$, and the outward intensities $I^+_{x\mu}(\tau_d)$ starting with the bottom boundary condition $I^+_{x\mu}(\tau_N) = S(\tau_N)$. In the integral form of the RT equation we assume that the line source function $S(\tau)$ has cubic behavior between successive depth points. The obtained intensities are then used for the computation of the relevant angle and frequency integrated moments and the iteration factors as their ratios. Therefore, the iteration factors are angle and frequency independent, defined for each line as a whole. They are used as the known coefficients to close the moments of the RT equation (for each line transition) that are to be solved simultaneously with the SE equations (for each level population) to update the solution in the second part of each iteration. At this step we have to deal with a strongly non-linear problem. The solution of the coupled non-linear equations can be found either by the linearization of the relevant equations or by their "preconditioning" (by use of an assumption that makes the SE equations linear, hence providing their linear coupling with the RT equation moments).

3.1. The iteration factors

In order to close the moments of the RT equation, we used two families of iteration factors, introduced in Paper I. For clarity and completeness, here we shall remind in brief of their definitions.

To obtain the frequency integrated mean intensity J_φ, which is implicitly contained in the corresponding line source function, we have to integrate the RT equations over both angles and frequencies. For each line frequency the first- and the second-order $\mu-$moments of Eq. (1) are given by

$$\frac{dH_x}{d\tau} = \varphi_x(J_x - S),$$

$$\frac{dK_x}{d\tau} = \varphi_x H_x. \tag{7}$$

By applying the operators $\int \varphi_x^2\{\ldots\}\,dx$ and $\int \varphi_x\{\ldots\}\,dx$ to the above two equations, respectively, for each line transition we obtain one system of two first-order moment equations:

$$\frac{dH_{\varphi^2}(\tau)}{d\tau} = J_{\varphi^3}(\tau) - \varphi^3 S(\tau),$$

$$\frac{dK_\varphi(\tau)}{d\tau} = H_{\varphi^2}(\tau), \tag{8}$$

i.e. one second-order differential equation of the form:

$$\frac{d^2K_\varphi}{d\tau^2} = J_{\varphi^3}(\tau) - \varphi^3 S(\tau). \tag{9}$$

Here we used the following notation for the intensity moments (Q stands for J, H, K) and for the profile moments:

$$Q_{\varphi^n}(\tau) = \int_{-\infty}^{\infty} \varphi_x^n Q_x\,dx, \quad \varphi^n = \int \varphi_x^n\,dx, \tag{10}$$

respectively.

The multilevel atom problem differs from the two-level-atom case in that the line source function $S(\tau)$ in Eq. (9) depends, via Eqs. (2) and (3), on the J_φ's of all the other line transitions in an implicit and non-linear way. As we shall discuss in detail in the next section, we have two possibilities to make the coupling of two sets of Eqs. (9) and (3), linear. Whichever we use, the introduction of some scalar closure relationships among the unknown intensity moments (J_φ, K_φ, H_{φ^2} and J_{φ^3}) is necessary.

The first family of iteration factors contains the most straightforward closure relations. Besides the generalized (frequency independent) Eddington factor

$$F = \frac{K_\varphi}{J_\varphi}, \tag{11}$$

it includes the factor

$$f_J = \frac{J_{\varphi^3}}{J_\varphi} \tag{12}$$

that relates the photons in the core (J_{φ^3}) to the photons of the entire line (J_φ). Using the factors (11) and (12) we can re-write Eq. (9) in the following form:

$$\frac{d^2K_\varphi}{d\tau^2} = \frac{f_J(\tau)}{F(\tau)} K_\varphi(\tau) - \varphi^3 S(\tau). \tag{13}$$

Apart from the Eddington factor (11), the second family includes the factors that account for the two-stream model of the radiation field and the non-local character of the radiative transfer. In the formal solution we treat separately the outgoing $I_{x\mu}^+(\tau)$ and incoming $I_{x\mu}^-(\tau)$ radiation field intensities and we remove the known, local and "passive in transfer" photons $I_0^\pm(\tau)$. We iterate only on the ratios of the non-local components of the radiation field $\tilde{I}_{x\mu}^\pm(\tau)$:

$$\tilde{I}_{x\mu}^+(\tau) = I_{x\mu}^+(\tau) - I_0^+(\tau) = I_{x\mu}^+(\tau) - S(\tau),$$

$$\tilde{I}_{x\mu}^-(\tau) = I_{x\mu}^-(\tau) - I_0^-(\tau) = I_{x\mu}^-(\tau) - S(\tau)(1 - e^{-\tau\varphi_x/\mu}), \tag{14}$$

thus carrying on, from one iteration to the next one, lesser amount of information.

Thus the factors of the second family are defined as follows:

$$\alpha^\pm = \frac{\tilde{J}_{\varphi^3}^\pm}{\tilde{J}_\varphi^\pm}, \quad \theta^\pm = \frac{\tilde{H}_{\varphi^2}^\pm}{\tilde{J}_\varphi^\pm}, \tag{15}$$

and used to put Eq. (9) in the form:

$$\frac{d^2K_\varphi}{d\tau^2} = \frac{f_J(\tau)}{F(\tau)} K_\varphi(\tau) + f_H(\tau)\frac{dK_\varphi}{d\tau} - (f_J(\tau) - f_S(\tau))S(\tau). \tag{16}$$

The coefficients f_J, f_H and f_S are related to the factors (15) in a simple way. The coefficient f_J plays a role of diffusion coefficient, f_H is a measure of the anisotropy of the radiation field and f_S reproduces the kinetic behavior of the transfer process.

Once we get the RT moment equations (13) or (16) we have to solve them simultaneously with the SE equations (3) in the second part of each iteration to get the improved values of the source function $S(\tau)$.

In our computations we used both families of the iteration factors but, in order to present two methods to solve the coupled RT and SE equations, for the sake of simplicity in the following we use the first IFs family only.

3.2. Non-linear coupling of RT and SE equations

3.2.1. Linearization

The first way to solve the above equations is to rewrite the second-order differential RT moment equations as difference equations and to linearize them in a similar way as first proposed by Auer and Mihalas [4]. We expand to the first order all the relevant variables x around their current estimates x_0, obtained in the previous iteration: $x = x_0 + \delta x$. For each line transition and for each of $N-2$ depth points we get a linearized RT moment equations (13) in the following form:

$$\begin{aligned}
&\frac{1}{\Delta\tau_d\Delta\tau_{d-1/2}}\delta K_{\varphi,d-1} - \frac{1}{\Delta\tau_d}\left(\frac{1}{\Delta\tau_{d-1/2}} + \frac{1}{\Delta\tau_{d+1/2}}\right)\delta K_{\varphi,d} \\
&\quad + \frac{1}{\Delta\tau_d\Delta\tau_{d+1/2}}\delta K_{\varphi,d+1} - \frac{f_{Jd}}{F_d}\delta K_{\varphi,d} + a_d\delta\chi_{d-1} + b_d\delta\chi_d \\
&\quad + c_d\delta\chi_{d+1} + \varphi^3\left(\delta\eta_d\chi_d - \frac{\eta_d\delta\chi_d}{\chi_d^2}\right) = \beta_d + \frac{f_{Jd}}{F_d}K_{\varphi,d} - \varphi^3\frac{\eta_d}{\chi_d},
\end{aligned} \tag{17}$$

where

$$a_d = \frac{\partial}{\partial \chi_{d-1}}\left\{\frac{d^2K_\varphi}{d\tau^2}\right\} = \frac{1}{\chi_d+\chi_{d-1}}\left[\gamma_d + \frac{1}{2}\beta_d\frac{\Delta\tau_{d-1/2}}{\Delta\tau_d}\right],$$

$$c_d = \frac{\partial}{\partial \chi_{d+1}}\left\{\frac{d^2K_\varphi}{d\tau^2}\right\} = \frac{1}{\chi_d+\chi_{d+1}}\left[\alpha_d + \frac{1}{2}\beta_d\frac{\Delta\tau_{d+1/2}}{\Delta\tau_d}\right],$$

$$b_d = \frac{\partial}{\partial \chi_d}\left\{\frac{d^2K_\varphi}{d\tau^2}\right\} = a_d + c_d,$$

$$\alpha_d = \frac{K_{\varphi,d}-K_{\varphi,d+1}}{\Delta\tau_d\Delta\tau_{d+1/2}}, \quad \gamma_d = \frac{K_{\varphi,d}-K_{\varphi,d-1}}{\Delta\tau_d\Delta\tau_{d-1/2}}, \quad \beta_d = \alpha_d+\gamma_d,$$

$$\Delta\tau_{d-1/2} = \tau_d - \tau_{d-1},$$

$$\Delta\tau_{d+1/2} = \tau_{d+1} - \tau_d,$$

$$\Delta\tau_d = \tfrac{1}{2}(\Delta\tau_{d-1/2}+\Delta\tau_{d+1/2}).$$

The linearized equations (17) are to be solved for the unknown corrections of the frequency integrated second order μ- moments of the radiation field intensities, δK_φ. To do that we express the changes in absorption and emission coefficients, $\delta\chi$ and $\delta\eta$, in terms of the changes in level populations (δn_i and δn_j) of a given transition ij:

$$\delta\chi_d = \sigma_0^{ij}\left(\delta n_{id} - \frac{g_i}{g_j}\delta n_{jd}\right), \quad \delta\eta_d = \frac{2hv_{ij}^3}{c^2}\sigma_0^{ij}\frac{g_i}{g_j}\delta n_{jd}, \tag{18}$$

where

$$\sigma_0^{ij} = \frac{hv_{ij}}{4\pi}B_{ij}\frac{1}{\Delta v_D}. \tag{19}$$

Now we can express the changes in the level populations in terms of δK_φ (i.e. $\delta J_\varphi = \delta K_\varphi/F$) by means of the following expressions:

$$\delta n_i = \sum_{kl}\frac{1}{F^{kl}}\frac{\partial n_i}{\partial J_\varphi^{kl}}\delta K_\varphi^{kl}, \quad \delta n_j = \sum_{kl}\frac{1}{F^{kl}}\frac{\partial n_j}{\partial J_\varphi^{kl}}\delta K_\varphi^{kl}, \tag{20}$$

with

$$\frac{\partial\overline{n}}{\partial J_\varphi} = -\mathbf{P}^{-1}\left(\frac{\partial\mathbf{P}}{\partial J_\varphi}\cdot\overline{n}\right) \tag{21}$$

obtained by linearizing equation (6). Substitution of the expressions for $\delta\chi_d$, $\delta\eta_d$, i.e. δn_i, δn_j, into Eqs. (17) yields the following system of coupled equations for the corrections δK_φ only

$$-A_d\delta K_{\varphi d-1} + B_d\delta K_{\varphi d} - C_d\delta K_{\varphi d+1} = L_d. \tag{22}$$

At the surface ($d=1$) and at the bottom ($d=N$) of the atmosphere we use the linearized form of the boundary conditions

$$\left(\frac{dK_\varphi}{d\tau}\right)_{\tau=\tau_d} = p_d + q_d K_\varphi(\tau_d). \tag{23}$$

Proceeding from the second equation (8) and taking that the intensity at the surface is $I^-_{x\mu}(\tau_1)=0$ and that at the bottom $I^+_{x\mu}(\tau_N)=S(\tau_N)$, we have

$$p_1 = 0, \quad q_1 = \gamma_1,$$

$$p_N = -\frac{\gamma_N}{2}\left[K\varphi^+(\tau_N) - \frac{1}{\gamma_N}H^+_{\varphi^2}(\tau_N)\right], \quad q_N = \gamma_N, \tag{24}$$

where the ratios:

$$\gamma_1 = \frac{H_{\varphi^2}(\tau_1)}{K_\varphi(\tau_1)} = \frac{H^+_{\varphi^2}(\tau_1)}{K^+_\varphi(\tau_1)} \quad \text{and} \quad \gamma_N = \frac{H^-_{\varphi^2}(\tau_N)}{K^-_\varphi(\tau_N)} \tag{25}$$

are computed at the first step of each iteration together with the iteration factors.

The tridiagonal system (22) is solved by the standard Gaussian elimination consisting of forward–backward recursion sweep. Its solution satisfies both the linearized transfer and the rate equations. At each depth point we have NT linearized RT equations, where NT is the number of line transitions. Hence, each element of the tridiagonal system is either $NT\times NT$ matrix or a vector of length NT. Let us note here that, compared to the complete linearization method of Auer and Mihalas [4] where the matrices of dimensions $(NF\times ND)\times(NF\times ND)$ (or $NF\times NF$ if VEFs are used) have to be inverted, now we have to invert the $NT\times NT$ matrices only.

The corrections δK_φ obtained by solving (22) are used to update the current values of the K_φ's and to compute the new values of the J_φ's through the Eddington factor (11). At the end of each iteration, with the new J_φ's we compute the improved values of the level populations from the SE equations with which we enter the next iteration step. The iterative procedure is terminated when the prescribed convergence criterion is achieved.

The level populations used in the solution of the coupled equations are those obtained in the previous iteration and corrected by one Λ iteration after the formal solution. Hence, the procedure within one iteration step is as follows: (i) the level populations (i.e. $S^{ij}(\tau)$) from the previous iteration are used in the formal solution of the RT equation to obtain the radiation field intensities, their moments and the iteration factors, (ii) with the computed J_φ^{ij} we re-compute level populations from the SE equations, (iii) together with the iteration factors, these level populations are then used in the solution of the coupled linearized RT and SE equations to obtain δK_φ^{ij}, and (iv) with δK_φ^{ij} we compute the new values of J_φ^{ij} and from the SE equations the updated values of the level populations (i.e. $S^{ij}(\tau)$) that enter the next iteration step.

3.2.2. Modification of the SE equations ("preconditioning")

In another approach to the simultaneous solution of the two systems of equations (RT and SE), certain approximation is used in the SE equations that makes the coupling linear. As well-known a way to transform the original non-linear equations into the linear ones is to take some quantities from the previous iteration as known. All the iterative methods developed to solve the RT problems assume, during the formal solution of the RT equation (at the beginning of each iteration step) that all the line absorption coefficients are known from the previous iteration. Here, we employ this assumption, i.e. we use the old (from the previous iteration) level populations $\{n^o\}$, not only in the formal solution of the RT equation, but also in the line-opacity-like terms of the SE equations (see e.g. [15,40]). This enables the level populations and, consequently, the relevant line source function, to be expressed as a linear function of the full set

of radiation field mean intensities in all line transitions (as described by Crivellari et al. [40]).

In order to make the SE equations (3) linear, let us first rewrite them by grouping the terms induced by the radiation field (both absorptions and stimulated emissions) in the right-hand side. Assuming that the line opacities are known, we modify the rate equations in such a way that only the coefficients of the terms J_φ^{ij} (which are the corresponding line absorption coefficients to the constant factor $h\nu/4\pi$) contain old (known) level populations. Thus, the modified (linear) SE equations have the following form (see [40]):

$$\sum_{i<j} C_{ij} n_i + \sum_{k>j} (C_{kj} + A_{kj}) n_k - \left[\sum_{i<j} (C_{ji} + A_{ji}) + \sum_{k>j} C_{jk} \right] n_j = -\sum_{i<j} (n_i^o B_{ij} - n_j^o B_{ji}) J_\varphi^{ij} + \sum_{k>j} (n_j^o B_{jk} - n_k^o B_{kj}) J_\varphi^{kj}. \quad (26)$$

Eqs. (26) can be put in the concise form:

$$\mathbf{U} \cdot \overline{n} = \overline{f}, \quad (27)$$

where the elements of the matrix $\mathbf{U}$ (of size $NL \times NL$) contain only the spontaneous emission A_{ji}, and the inelastic electron collision C_{ji} terms (except in the last row that contains 1's due to the particle conservation Eq. (5)), while the vector $\overline{f}$ contains the net radiative rates $(n_i^o B_{ij} - n_j^o B_{ji}) J_\varphi^{ij}$. By inverting the matrix $\mathbf{U}$ it is possible to express new (unknown) level populations n_j as linear functions of yet unknown mean intensities in all line transitions:

$$n_j = n_j^c + \sum_{kl} \Gamma_j^{kl} J_\varphi^{kl}. \quad (28)$$

In Eq. (28) the terms n_j^c, given as

$$n_j^c = u_{j,NL}^{-1} \cdot n_{\text{total}}, \quad (29)$$

contain only A_{ji}, C_{ji} and n_{total} that are known for a given atomic and atmospheric model, while the matrix elements Γ_j^{kl} contain not only the elements u_{jl}^{-1} of the inverse matrix but also the old level populations $\{n^o\}$ via the coefficients $n_i^o B_{ij} - n_j^o B_{ji}$.

With the known absorption coefficients, from Eqs. (2) and (28) it is easy to derive the similar linear relations for each line source function S^{ij} in terms of the full set of radiation fields in all NT line transitions:

$$S^{ij} = S_c^{ij} + \sum_{kl} \sigma^{ij,kl} J_\varphi^{kl}. \quad (30)$$

Here

$$S_c^{ij} = \frac{A_{ji}}{n_i^o B_{ij} - n_j^o B_{ji}} n_j^c,$$

$$\sigma^{ij,kl} = \frac{A_{ji}}{n_i^o B_{ij} - n_j^o B_{ji}} \Gamma_j^{kl}. \quad (31)$$

By means of the Eddington factor it is straightforward to write the linear relations between S^{ij} and the full set of the K_φ's

$$S^{ij} = S_c^{ij} + \sum_{kl} \frac{\sigma^{ij,kl}}{F^{kl}} K_\varphi^{kl}. \quad (32)$$

The modified SE equations provide a situation analogous to that of the two-level-atom line transfer problem in which the linear SE equations are solved together with the RT equation moments. Substituting Eq. (32) into the RT moment Eq. (13) rewritten in the difference equation form, we finally get the following system:

$$\frac{1}{\Delta\tau_d \Delta\tau_{d-1/2}} K_{\varphi d-1} - \frac{1}{\Delta\tau_d} \left(\frac{1}{\Delta\tau_{d-1/2}} + \frac{1}{\Delta\tau_{d+1/2}} \right) K_{\varphi d} + \frac{1}{\Delta\tau_d \Delta\tau_{d+1/2}} K_{\varphi d+1} - \frac{f_{Jd}}{F_d} K_{\varphi d} + \varphi^3 \sum_{kl} \frac{\sigma_d^{ij,kl}}{F_d^{kl}} K_{\varphi d}^{kl} = -\varphi^3 S_{c,d}. \quad (33)$$

This system can be expressed in the tridiagonal form and solved together with the boundary conditions (23) by the standard Gaussian elimination procedure. The improved values of the K_φ's satisfy the RT and SE equations simultaneously.

Let us briefly summarize the above procedure. At the beginning of each iteration step, the level populations given (in the first iteration) or obtained from the previous iteration step are used in the formal solution of the RT equation and, hence, in the computation of the iteration factors. These populations $\{n^o\}$ also enter the modified SE equations (26) and, consequently, the coefficients of the linear relations (32) between each line source function S^{ij} and the radiation fields in all NT line transitions. By substituting Eq. (32) in the RT moment equations (13) for the first family of iteration factors, i.e. into the RT moment equations (16) for the second family, we compute the improved values of the K_φ's and, hence, of the J_φ's. With these new mean intensities the original SE equations are solved, resulting in the new values of level populations that enter the next iteration step.

4. Numerical tests and results

The iterative procedures proposed above were tested on the standard benchmark model for the multilevel atom problems given by Avrett and Loeser [2]. They analyzed spectral line formation by three-level hydrogen atoms in a plane-parallel, semi-infinite isothermal ($T = 5000$ K) atmosphere, with no background opacity, giving the solutions for two cases: with constant collisional deexcitation rates $C_{ji} = 10^5\ \text{s}^{-1}$ (Case 1), and with collisional rates decreasing rapidly near the surface $C_{ji} = 10^5(1-0.99\exp(-0.1\tau_{12}))\ \text{s}^{-1}$ (Case 2).

We solved these test cases using both families of iteration factors (F1 and F2) and both methods for the solution of non-linear coupling of the RT and SE equations (linearization (L) and the modification of the SE equations (M)). Thus we obtained and analyzed four solutions: F1-L, F1-M, F2-L and F2-M.

In all these solutions the iterative procedure was initialized by assuming equilibrium (LTE) values of the level populations. In order to provide stable convergence, the relaxation was needed: $Q^{(i)} = (1-r)Q_{\text{out}}^{(i)} + rQ_{\text{in}}^{(i)}$, where $Q_{\text{in}}^{(i)}$ and $Q_{\text{out}}^{(i)}$ are the input and the current values of the variable Q in the i-th iteration ($Q_{\text{in}}^{(i)} = Q^{(i-1)}$), and $0 < r < 1$ is the relaxation parameter. The fact that the IF method

may need the under-relaxation when applied to a physically simple, but numerically difficult problem was already known from the analysis of its convergence properties given in Paper I. For small departures from LTE the relaxation is not necessary, but for larger departures the under-relaxation (found by a trial-and-error approach, but usually either 0.5 or 0.75) is needed to slow down the convergence. In all four solutions considered here, $r=0.75$ was used. Let us point out (as stated in Paper I) that in some more realistic applications of the method, the relaxation is not necessary.

The properties of the iterative procedures are analyzed by calculating at each iteration step i the following quantities [18]:

the maximum relative change

$$R_c^i = \left|\frac{S^i - S^{i-1}}{S^i}\right|_{\max}, \tag{34}$$

the maximum relative convergence error

$$C_e^i = \left|\frac{S^i - S^{\infty}}{S^{\infty}}\right|_{\max}, \tag{35}$$

and the maximum relative true error

$$T_e^i = \left|\frac{S^i - S^{\infty}_{\mathrm{REF}}}{S^{\infty}_{\mathrm{REF}}}\right|_{\max}. \tag{36}$$

Here, S^{∞} is the fully converged solution of the IFM obtained by a preliminary long run. Since the analytical solution of this benchmark problem is not known, the true accuracy of the IFM is expressed with respect to $S^{\infty}_{\mathrm{REF}}$—the fully converged "exact" solution obtained with a well-tested RT code. In this paper we used the FBILI method [26] as the reference (REF) one, primarily because we could run both methods (FBILI and IFM), straightforwardly getting the solutions for different choices of input parameters, and because the FBILI solutions differ with respect to the solutions of Avrett and Loeser [2] by less than 3%. Note, however, that Avrett and Loeser solutions are given only for the spatial grid with three depth points per decade. We also compared the convergence rate of the IFM with that of the MALI method, using the results given in [15] for the same benchmark problem.

The computations were performed using 23 Avrett and Loeser frequencies, four Gauss–Legendre angles and three different grids in optical depth (with 3, 6 and 9 points per decade), from $\tau=10^{-3}$ to 10^{14}. The coarser grids are chosen so that their points coincide exactly with some of those corresponding to the finest grid. The comparison of the solutions obtained by the IFM in each particular spatial grid with the FBILI "exact" solutions obtained with the finest grid, enabled us to investigate the dependence of its accuracy on the grid refinement.

4.1. The first family of iteration factors

Firstly we used the most simple family of iteration factors, defined by Eqs. (11) and (12), in order to check the validity of the proposed procedures.

By using the linearization to solve the coupled RT and SE equations (F1-L) the convergence was not achieved for Avrett and Loeser's original test case (with the collisional deexcitation parameter $C_{ji}=10^5\ \mathrm{s}^{-1}$). The solution was, however, obtained for smaller departures from LTE. Thus, for example, with $C_{ji}=10^6\ \mathrm{s}^{-1}$ the procedure converged in only 10 iterations with the true accuracy of 1% when the finest spatial grid (with 9 points per decade) was used. This result proved the correctness of our method and confirmed the existence of stability problems with the most straightforward closure relations, already known from Paper I.

The use of the modified SE equations (F1-M) led to the "exact" solution of the original test case in a very small number of iterations. As an example, only eight iterations were needed to reach the maximum relative change R_c of 1% and the maximum relative true error T_e of only 2% with a coarser grid of 6 points per decade. In Fig. 2 we show the behavior over iterations of the first family of factors, F and f_J, for all three line transitions. After a few iterations the factors reach their "exact" values. At great optical depths they have their equilibrium values, so that the generalized Eddington factor F approaches $\frac{1}{3}$, while f_J tends to the value of φ^3.

The behavior of the source functions over iterations for the three hydrogen spectral lines is presented in Fig. 3, together with the corresponding FBILI solutions. It is interesting to note the well-known $\sqrt{\varepsilon}B$ law (where ε is the standard NLTE parameter and B is the Planck function) at the surface for the strong resonance Lyman α line, for which even the two-level atom model is quite appropriate. As can be seen from the plots, already after the first iteration the solution attains the correct thermalization length. This is the most important difference with respect to the simple Λ iteration procedure. Λ iteration corrects the solution at each iteration step only within a unit optical path, so that in the early stages of iteration it gives no indication where the thermalization takes place. Here, the corrections are made simultaneously throughout the entire medium owing to the use of the iteration factors. Being defined as the ratios of the relevant intensity moments, the IFs depend only slightly on the poor (equilibrium) initial estimates of level populations (i.e. source functions) and reach their almost exact values already in the first few iterations. The line source functions are thus largely corrected at the very beginning of the iterative procedure, reaching the accuracy of 2% in a few iterations. Note, however, that the maximum relative change $R_c \le 10^{-3}$ could not be achieved.

Thus, we were again faced with the fact, known from Paper I, that the most straightforward closure relation, although providing an extremely fast and accurate solution, does not satisfy completely the requirement of stability in the cases of large departures from LTE. This problem was solved by the use of more general closure relationship as is shown below.

4.2. The second family of iteration factors

The improved iteration factors family, Eq. (15), derived from the best numerical simulation of the transfer process, led to the fast, exact and more stable solutions

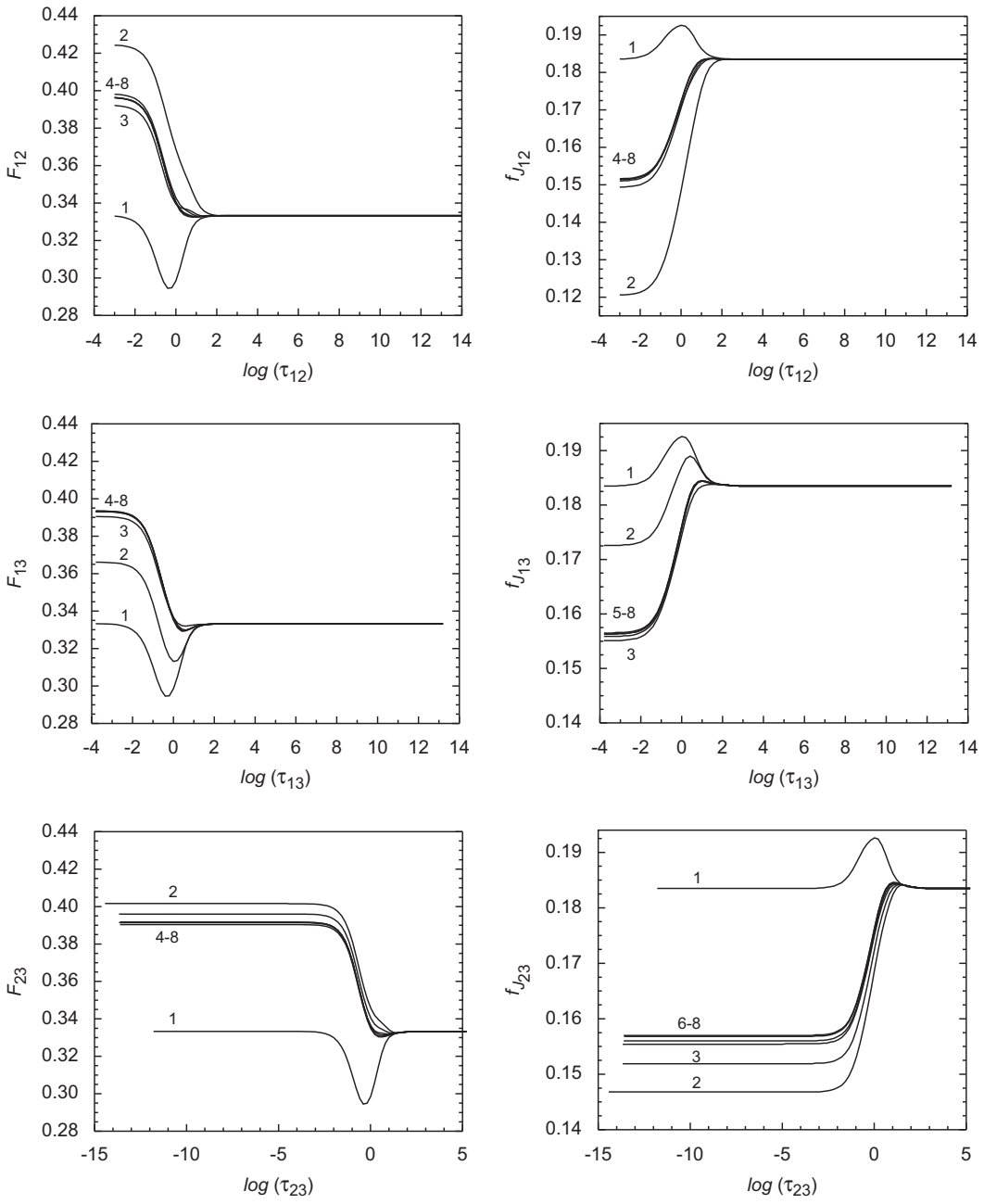

Fig. 2. The variation of the iteration factors F and f_J for three hydrogen line transitions, obtained by the use of modified SE equations (F1-M) for Avrett and Loeser Case 1 in the indicated number of iterations.

with both methods for solving the non-linear coupling of the RT and SE equations.

In the procedure based on linearization (F2-L) when iterations started from the LTE populations, a few negative radiation field intensities occurred in the first iteration due to large corrections near the surface; these, however, did not affect the overall procedure, which resulted in positive mean intensities in all subsequent iterations. The procedure remained stable up to the maximum relative corrections R_c of about 10^{-6}, while the maximum convergence error of 1% was reached in about 15 iterations.

The instabilities that led to negative intensities in the first iteration were removed by initializing the procedure with the independent solutions of the two-level atom problems, taking into account only the spectral lines of the Lyman series, from which the solution for the subordinate line can be easily derived. It was even not necessary to take the final solutions of the two-level atom problems, but the solutions obtained in the second iteration, since they are closer to the final solution of the multilevel problem than the equilibrium ones. The convergence was rapid, reaching the maximum relative change R_c of 1% in only 12 iterations, and the maximum convergence error C_e of 1% also in about 15 iterations (see Table 1).

Having obtained the exact, stable and fast solutions we investigated the accuracy and the convergence properties

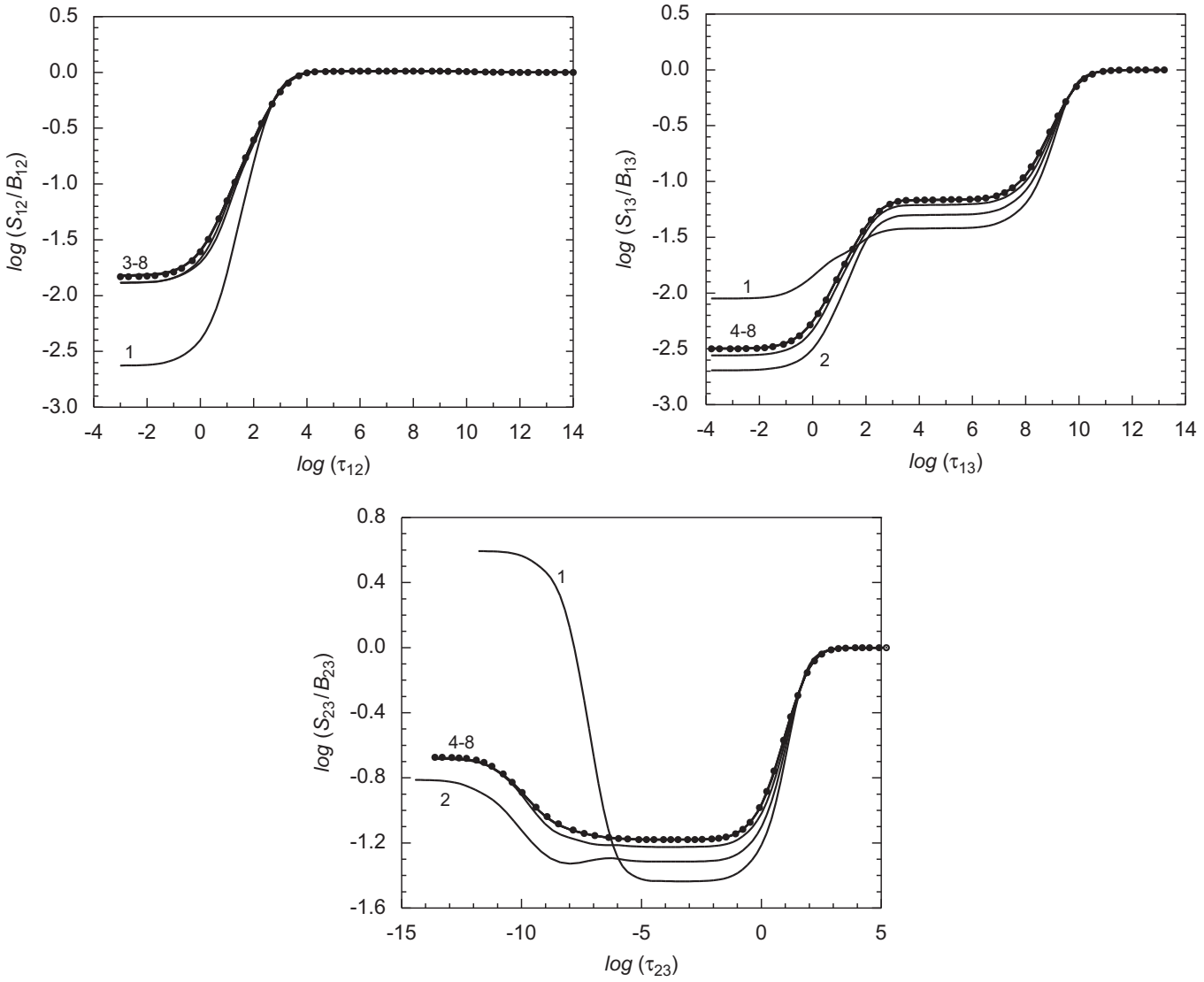

Fig. 3. The convergence of the source function for three line transitions using the first family of the factors and the modified SE equations (F1-M) for Avrett and Loeser Case 1 in the indicated number of iterations. The solutions obtained with FBILI are given by dots.

Table 1
Number of iterations needed by the IFM (using procedure F2-L) to satisfy various convergence criteria: (a) $R_c \le 10^{-2}$, (b) $R_c \le 0.1T_e(\infty)$, (c) $C_e \le 10^{-2}$ and (d) $C_e \le 10^{-4}$ for four spatial grids (N_τ is the number of depth points per decade).

N_τ	$R_c \le 10^{-2}$	$R_c \le 0.1T_e$	$C_e \le 10^{-2}$	$C_e \le 10^{-4}$
Case 1				
3	12	13	14	28
6	12	15	14	27
9	13	21	16	32
18	13	23	15	28
Case 2				
3	13	13	15	28
6	13	16	14	27
9	12	18	14	26
18	13	23	39	49

Above for Case 1, below for Case 2 of the three-level H atom benchmark problem [2].

of the method in more details. In order to investigate the dependence of the accuracy on the spatial grid resolution, we solved the test cases in three grids (with 3, 6 and 9 points per decade) and compared the solutions with the fully converged source functions obtained with the FBILI code in the finest spatial grid. The variation of the maximum relative true error T_e corresponding to these grids with the iteration number is shown in Figs. 4a and 5a for Avrett and Loeser Cases 1 and 2, respectively. One can see that after a rapid initial improvement T_e exhibits an asymptotic behavior with iterations, reaching the so-called truncation error $T_e(\infty)$ (a measure of the true accuracy) of about 9%, 3% and 1%, for the grids with 3, 6 and 9 points per decade, respectively. Let us note that the accuracy of 1% is usually considered as good enough when two different numerical codes are compared. Further increase in the grid resolution led to an even higher accuracy, so that

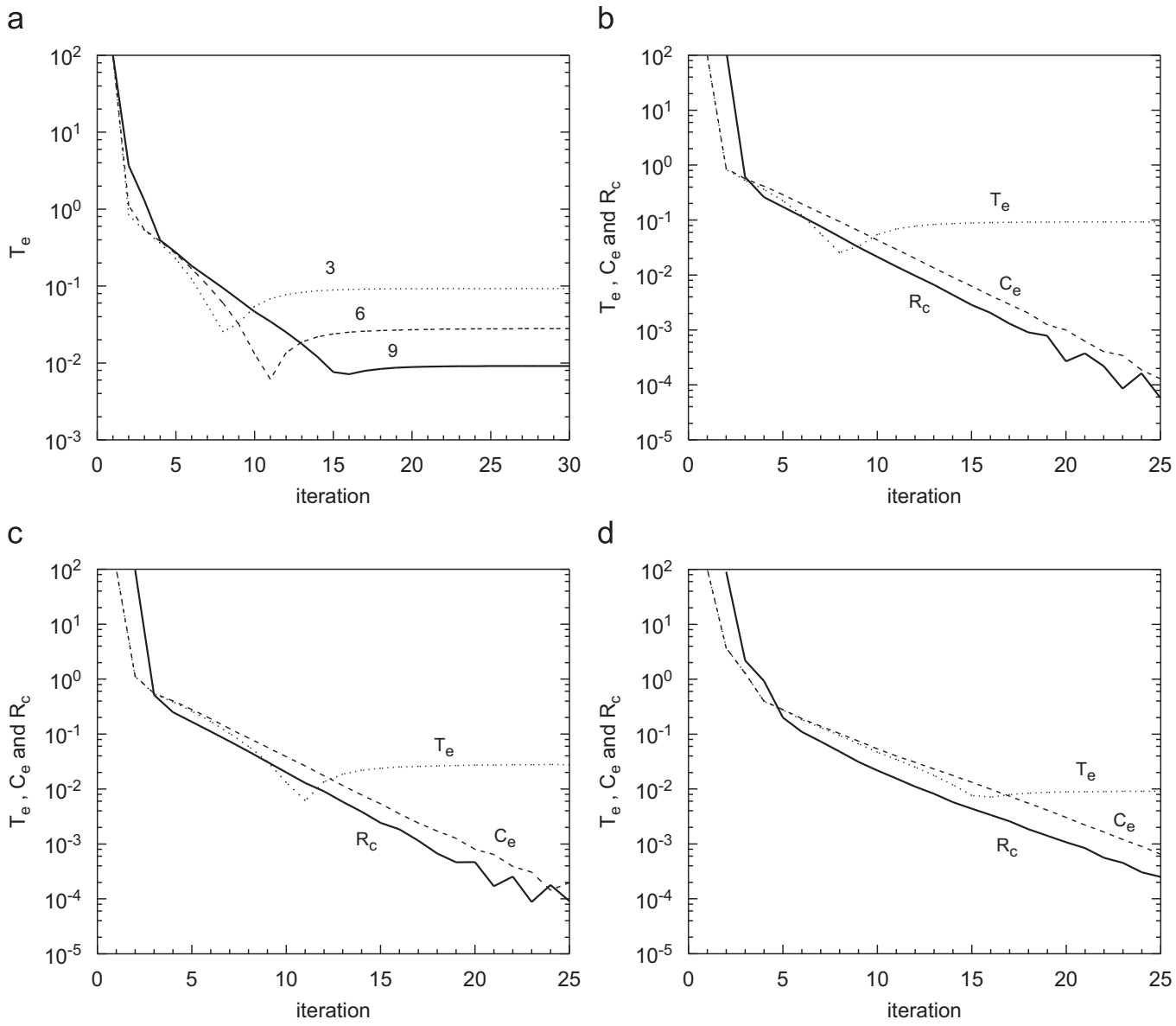

Fig. 4. (a) The maximum relative true error T_e for three spatial grids with the iteration number, (b)–(d) the maximum relative change R_c, the maximum relative convergence error C_e and the maximum relative true error T_e as a function of the iteration number for 3, 6 and 9 depth points per decade, obtained by the IFM, using the second family of factors and the linearization (F2-L), for Case 1.

with 18 depth points per decade the true accuracy of 0.25% was achieved.

For each of the three spatial grids used, in the panels (b)–(d) of Figs. 4 and 5 (for the Cases 1 and 2, respectively), we show the variations with the iteration number of the maximum relative change R_c and the maximum convergence error C_e (over all line transitions and all depth points in the atmosphere), together with the corresponding true error T_e. We see that the iterations can be stopped once the criterion $R_c < 0.1T_e(\infty)$ [18] is satisfied, as the further decrease in relative corrections does not increase the accuracy achieved any more.

From Figs. 4 and 5, one can also see that the convergence rate of the IFM is practically insensitive to the spatial grid used. This is also illustrated by Table 1 in which, for both test cases and for different spatial grids (including $N_\tau = 18$ as well), we display the number of iterations needed by the IFM code to reach: the stopping condition $R_c \leq 10^{-2}$ usually used in the literature (see, e.g. [1,21]), the criterion $R_c < 0.1T_e(\infty)$ (suggested in [18]), as well as $C_e \leq 1\%$ and $C_e \leq 0.01\%$ (as the measures of the method's internal accuracy). One can see that whatever the condition, the convergence rate is very high and insensitive to the spatial grid.

The use of the F2-M approach for the solution of this benchmark problem led to similar results. For the same spatial grids considered, the maximum relative true error T_e reached the same asymptotic values as in the F2-L solution. Convergence is achieved in a similar number of iterations, reaching, however, the maximum relative changes of only up to about 10^{-4}. The convergence properties of the Avrett and Loeser case 2 were almost identical to those of case 1.

As a further test, we applied our method to the CaII ion model with five bound levels, five radiative and 10

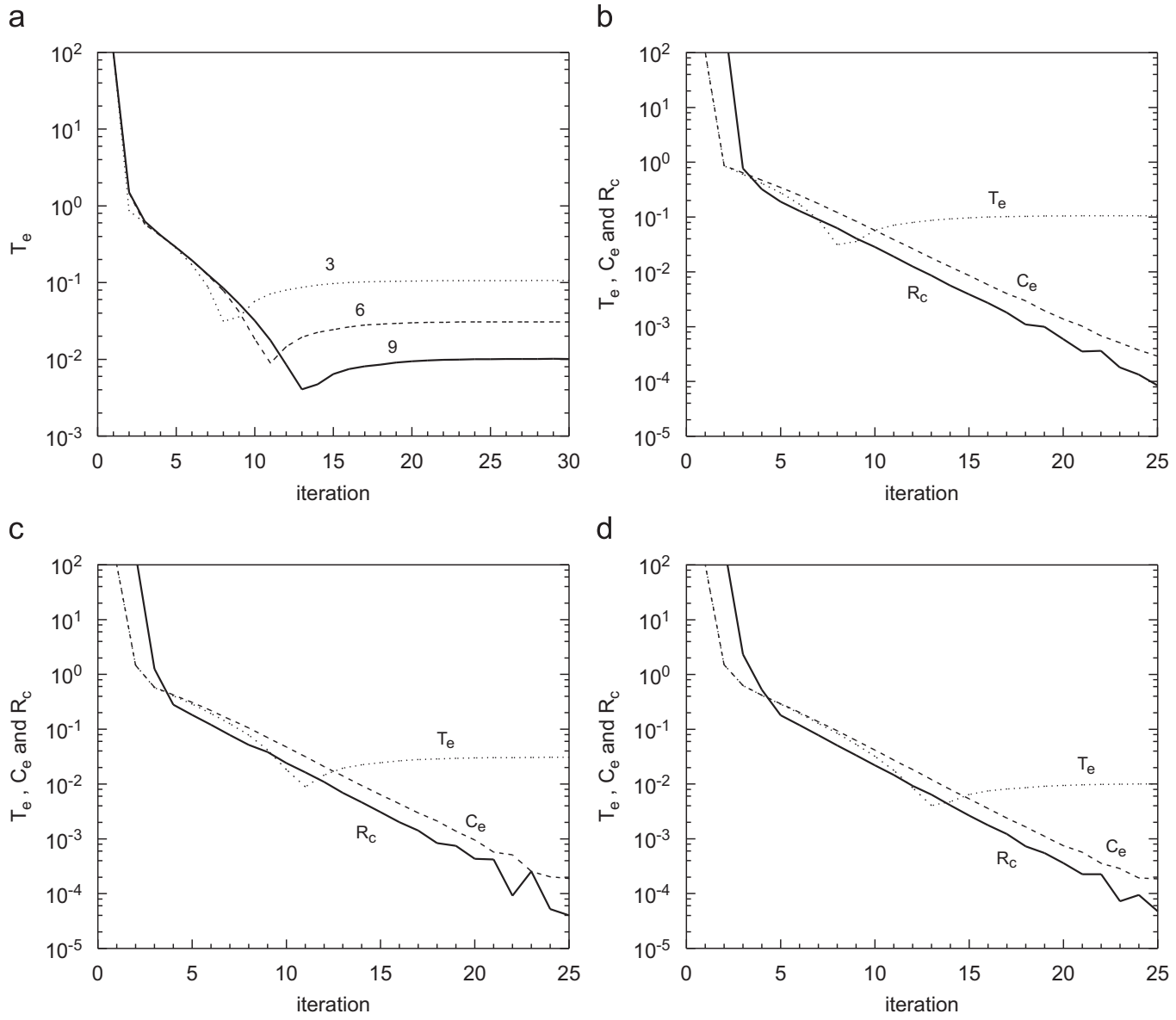

Fig. 5. Same as in Fig. 4, but for Case 2.

Table 2
Number of iterations needed by the IFM (for all four procedures) to reach a given maximum relative change in the solution of a five-level CaII test problem.

R_c	F1-L	F1-M	F2-L	F2-M
10^{-2}	9	6	7	7
10^{-3}	12	13	11	13
10^{-4}	15	30	13	30
10^{-5}	24	58	24	58

collisional transitions in an isothermal atmosphere at $T = 5000$ K, using the input parameters given in [8,25]. This test case was also solved with four runs, using both families of iteration factors and both methods for the solution of the non-linear coupling of the RT and SE equations. It was again initialized assuming LTE. The convergence properties are found to be generally similar to, and in some cases even better than, those of the three-level H atom test case. The accuracy grows at approximately the same rate with grid resolution. The convergence rates of the four solutions are summarized in Table 2. The results are given for 6 points per decade, but they coincide completely for the other grids used, demonstrating again the independence of the convergence rate on the grid resolution.

4.3. Convergence properties: comparison with other methods

In this section we shall compare the convergence rate and the total computational work of the IFM with those of some other methods. Our intention is not to argue that this approach is better or not than some other one, but rather to show that its further generalization to other

more realistic and more complex problems is fully justified.

Apart from the comparison with the FBILI method that we use as the reference one, we shall also compare the properties of our method with those given by Rybicki and Hummer [15], who solved the same benchmark problem [2] with the MALI method. Rybicki and Hummer used diagonal (D) and tridiagonal (T) approximate Lambda operators, without (N) and with Ng acceleration (A). They reported that with no acceleration a "true" accuracy of about 1% was obtained after about 80 iterations with the diagonal method (D/N) and after about 25 iterations with the tridiagonal method (T/N). By "true" accuracy Rybicki and Hummer meant the "true" relative error of maximum absolute size, based on the "exact" solution found by a preliminary long run with their fastest method (internal accuracy). This criterion corresponds to that defined by Eq. (20) in Auer et al. [18] or to the convergence error given by Eq. (35) of the present paper. The true accuracy that we used (Eq. (36)) was defined with respect to some other "reference" method (external accuracy). Having in mind that about 15 iterations are needed by the IFM to reach the internal accuracy of 1% (see Table 1), we see that the convergence rate of the IFM is higher than that of MALI by a factor of more than 5 with respect to the D/N, and by a factor of about 2 for the T/N method. Concerning MALI methods with acceleration, Rybicki and Hummer reported that an accuracy of 0.01% was obtained in 25 and 12 iterations, with D/A and T/A, respectively. The same accuracy is reached by the IFM after about 29 iterations, which is comparable with the number of iterations needed by the diagonal method, accelerated (D/A). Only the use of tridiagonal ALO with Ng acceleration (T/A) provided more rapid convergence than the IFM. It is, however, known that the optimal convergence of the iterative procedure using Ng acceleration depends on the optimal values of two control parameters: the iteration number at which the acceleration is turned on and the number of previous iterations used that require some preliminary numerical tests and analysis (see, e.g., the discussion on this topic in [15,21]). We want to stress that the IFM does not need any additional acceleration.

The above considerations, however, do not give us a complete insight into the efficiency of the IFM. Namely, the saving in the number of required iterations does not necessarily imply the saving in the total computational work (CW). It is necessary to compare the computing time per iteration and then to derive the conclusions about the total CW.

To do this, let us recall that at each iteration step the IFM requires the solution of a block tridiagonal system for NT transitions and the solution of the SE equations for NL level populations at each depth. Thus the computing time scales as $\approx N \times NT^3 + N \times NL^3$. The diagonal MALI method (as well as the FBILI method) requires the solution of the SE equations for NL populations at each depth, which scales in each iteration approximately as $\approx N \times NL^3$. The computing time for the tridiagonal MALI method, which requires the solution of a block tridiagonal system for the populations, also scales as $\approx N \times NL^3$. Therefore, there is an extra cost in the IFM of the $NT \times NT$ matrix inversions, which is, as we shall see, compensated by its high convergence rate.

Table 3
Computational work (CW) in seconds, the number of iterations required (iter) and the computation time per iteration (CPU/it) for the three-level H atom benchmark problem [2] as a function of the number of depth points per decade N_τ.

N_τ	Λ iteration	FBILI			IFM		
	CPU/it	CW	iter	CPU/it	CW	iter	CPU/it
3	0.0135	0.172	11	0.0156	0.422	23	0.0183
6	0.0264	0.438	15	0.0292	0.813	23	0.0353
9	0.0395	0.828	19	0.0436	1.469	28	0.0525

The results are obtained with an Intel(R) Pentium(R) Dual CPU at 2.2 GHz. The stopping criterion is $R_c = 10^{-4}$.

The cost per iteration of the above iterative methods can be expressed in terms of the CPU time per Λ iteration, which is known to be the shortest possible. Thus, for the sake of comparison of their total computational work we ran the classical Λ iteration, the IFM and the FBILI codes, bearing in mind that in the MALI D/N method the computing time per iteration is practically the same as that per classical Λ iteration. In all the codes the integral form of the RT equation and the same short-characteristics formal solver with the cubic representation of the source function between two successive depth points are used. In Table 3 for each chosen grid we show the CPU time per Λ iteration, as well as the total computational work, the number of iterations needed to reach the maximum relative change $R_c = 10^{-4}$ and the CPU time per iteration for the FBILI and the IFM. All three codes were run with the same discretization in angles, frequencies and depths. The condition $R_c = 10^{-4}$ is sufficient to claim that the convergence to the exact solution is achieved in all the chosen grids. We can see that the computing time per IFM iteration is about 20% longer than the computing time per FBILI iteration, and about 30% longer than the computing time per Λ iteration. We can also infer that, in terms of the total CW, the IFM is slower than the FBILI by a factor of 2. On the other hand, using the known convergence rates of the MALI and IFM (given in [15] and in this paper), we can conclude that the total computational work needed by the IFM is at least 4 times less than that needed by MALI to get the solutions of the same accuracy.

From Table 3 we can also see the dependence of the total computational work (CW) of the IFM on the grid spacing. It is known that the computational work of the MALI method with local approximate operator [15], as well as of all the methods based on Jacobi's iteration [13,18], scales approximately as $N_\tau \times N_\tau$ (N_τ—the number of depth points per decade), since both the CW of the formal solver and the number of iterations needed to reach the convergence scale with N_τ. The method based on Gauss–Seidel iterations scales as $N_\tau \times N_\tau/2$, the SOR-based technique as $N_\tau\sqrt{N_\tau}/2\sqrt{2}$, while the multilevel nonlinear multigrid methods scale as N_τ [23]. Note that, as pointed out by Trujillo Bueno and Fabiani Bendicho [22],

the Gauss–Seidel and SOR methods for radiative transfer applications can be easily implemented in such a way that the number of iterations required to reach convergence is actually an extra factor 2 smaller, as was done in practice by Trujillo Bueno and Manso Sainz [41] for the non-LTE polarization radiative transfer problem. From Table 3 we see that the CW of the IFM scales simply as N_τ, since the CPU time per iteration scales as N_τ and the number of iterations required to reach the given criterion is practically insensitive to the grid resolution.

The above considerations show that the convergence properties of the IFM (speed and accuracy) are comparable with those of the ALI methods. Moreover, two basic advantages of the IFM with respect to the ALI methods currently in use are: (1) extremely fast convergence with no need for an extra mathematical acceleration, and (2) there is no increase in the number of iterations with the grid resolution refinement.

On the other hand, we show that it is possible to define angle and frequency integrated iteration factors so that the dimensions of the problem are drastically reduced, not only for angles but also for frequencies. Hence, we see that this approach, similarly to the hybrid ones, combines good properties of the global CL approach (its high convergence rate) and of the ALI methods (computationally cheaper and faster per iteration). These conclusions explain and justify the motivation for our approach.

5. Conclusions

The method of iteration factors, developed in Paper I for the linear 2-level atom line formation problem, is in this paper extended to the multilevel atom case.

Besides the non-local coupling between the radiation field and the state of the gas that is inherent to all radiative transfer problems, the multilevel line formation has, from the mathematical point of view, the additional difficulty arising from the non-linear dependence of the atomic level populations (i.e. source functions) on the line radiation field intensities. Therefore, in comparison with the linear two-level-atom RT problem studied in Paper I, an additional computational effort is required for the simultaneous solution of the RT and SE equations, being now non-linearly coupled. We solve this problem in two ways: by linearization of the relevant equations and by modification of the SE equations that makes them linear.

In the first approach, in the difference-equation form of the RT moment equation we expand to the first order all the relevant variables and eliminate the changes in absorption and emission coefficients, i.e. the changes in level populations, by means of the linearized SE equations. The resulting system of equations contains the changes in the radiation field δJ_φ only. Its solutions satisfy both sets of equations, the RT and SE. In the second approach we use the linear form of the SE equations obtained assuming that the level populations in the line-opacity-like terms are known from the previous iteration. This enables to write the rate equations in a linear form and to express each line source function as a linear function of the radiation fields in all the relevant line transitions. Substitution of such modified SE equations into the RT equation moments results in the system for J_φ only, satisfying again both sets of equations simultaneously. Whichever approach is chosen, the RT equation moments are closed by the quasi-invariant iteration factors, computation of which leads extremely fast to an accurate solution.

In order to test the method and check its accuracy and efficiency we applied it to the well-known complete redistribution pure line-transfer problem for three-level hydrogen atoms in a constant property medium [2]. We compared our solutions with those obtained with some other methods used to solve the same kind of RT problems in order to investigate in more details its properties, advantages and limitations. We have shown that the use of iteration factors leads to a very fast convergence (in about 10–20 iterations) to the solution that differs by only 1–3% from the solutions obtained by other methods in the usual spatial grids, and even by about 0.25% in the same number of iterations with a high grid resolution of 18 depth points per decade. The generalization to the multilevel case confirmed again that the more refined factors are used, the better the convergence properties. The convergence is extremely rapid even though the iterative procedure is started with the corresponding equilibrium values and no additional acceleration is used. Very high convergence speed is not affected by the refinement of the grid resolution, i.e. the convergence rate is practically insensitive to the spatial grid, so that the total computational work scales linearly with the number of grid points. As an additional check we applied the IFM to the solution of a 5-level CaII ion model, obtaining similar, and in some cases even better results.

By applying the IFM to the simplest, from the physical and mathematical point of view, but not so simple from the numerical point of view, test problem we aimed at investigating its accuracy and convergence properties. For the sake of clarity and self-consistency of the analysis, we postpone its extension to physically more general cases (line formation with background continuum in a variable property media) to the forthcoming Paper III (as announced already in Paper I). Let us emphasize that the IFM, as already shown in Paper I, has better convergence properties, i.e. higher convergence rate and greater stability (with no relaxation needed) when applied to physically more complex, but numerically more stable problems.

In general, the method of iteration factors is problem dependent as the choice of the IFs as good quasi invariants is determined by the physics of the problem itself and the mathematical structure of the equations one has to solve. However, this potential disadvantage is amply compensated by its very fast convergence to the exact solution with no need for an extra acceleration. Therefore, its overall convergence properties are similar to those of the global CL method. On the other hand, our factors, being defined for each spectral line as a whole, drastically reduce the need for large memory storage and a cost per iteration, thus successfully removing the main drawback of the CL approach. The fact that the total computational work of the IFM scales linearly with the number of grid

points is an advantage with respect to the ALI methods currently in use.

There is no doubt that an impressive progress is made in the last two decades in the RT numerical modelling and that quite robust ALI methods are already employed in solving various and complicated physical problems. However, the study and examination of other possible solutions is still actual, as it is always of interest and importance to have as many independent methods as possible in order to check and verify the obtained results. The accuracy and convergence properties of the IF method are so good that its study, further development and use are fully justified.

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