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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