THE STELLAR ATMOSPHERE PHYSICAL SYSTEM II. AN OPERATIVE SEQUENTIAL ALGORITHM TO SOLVE THE STELLAR ATMOSPHERE PROBLEM

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SUMMARY: In this paper, the second and the last of the series, we present a sequential algorithm to solve the stellar atmosphere problem that may serve as a paradigm for the solution of more general non-linear and non-local problems. The Iteration Factors (IF) Method is applied to achieve a solution of the radiative transfer equations, consistent with the radiative equilibrium constraint.

Key words. Stars: atmospheres – Methods: numerical – Radiative transfer

1. INTRODUCTION

Many physical problems are *non-linear* in character. Their direct numerical solution may be found in principle for a limited number of instances; however, very often such a solution turns out to be unfeasible in the practice. Therefore, we must assume that, but for a very few exceptions, the problems posed by non-linear physics necessarily require iterative numerical procedures for their solutions. On the other hand, a direct solution of *linear* problems is always possible in principle. Nevertheless, in many cases the huge dimension of the problem makes a direct solution incompatible with the standards of accuracy, stability and reliability required. Hence the need of looking for efficient iterative algorithms that fulfil the foregoing standards also in the case of linear problem. An exhaustive discussion of iterative methods for the solution of radiative transfer problems, both linear and non-linear, is contained in Simonneau and Crivellari (2002).

In this second paper of the series we study a simplified but significant case of stellar atmosphere modelling to be considered as a paradigm for non-linear problems. Our aim is to illustrate by means of a concrete example how analysis of the physics of the problem paves the way towards an operative numerical algorithm for its solution. The underlying principles and the stellar atmosphere problem were introduced in Paper I of this series (Crivellari 2018). After an outline of the Iterative Sequential Approach (Section 2) and a definition of strong and weak couplings (Section 3), we specify in Section 4 the fundamental equations relevant to the case study under consideration here. The kernel of the present paper consists of the introduction of an iterative sequential algorithm for the solution of the problem. Section 5 presents an analysis of this approach. On this basis in Section 6 we consider the reasons of the failure of both a straight iterative sequential procedure and its improved version. The way of getting out of the impasse is shown in Section 7 where the Iteration Factors Method is introduced and discussed. Concluding remarks are drawn in Section 8.

2. AN ITERATIVE SEQUENTIAL APPROACH

In Section 7.2 of Paper I we presented and discussed the fundamental equations of the stellar atmosphere problem. We stressed there that the coupling of the above equations brought about by the influence of the physical variables on the transport coefficients that characterize the radiative transfer (RT) equations renders the problem non-linear. A way to get rid of this difficulty may be a global approach based on the linearization of all the relevant equations. As a matter of fact, such an approach is widely in use for the computation of stellar atmosphere models. This complete linearization technique, however, has one severe drawback: it implies the storage and successive inversion of matrices of huge dimensions (of the order of 10^4 and more), with the consequent high risk of both destructive numerical instabilities and loss of the numerical accuracy required.

Moreover, a consideration of physical character casts doubts on the complete linearization technique as an operative method of solving the stellar atmosphere problem. As explicitly stated in Mihalas (1978), this method rests upon the assumption that no one variable is more fundamental than any other. This 'egalitarian' principle is, however, refutable because not only are the different phenomena characterized by very different height scales but also, and above all, the interactions among the different components of the whole physical system produce effects of different degrees of importance, and should accordingly be arranged in a hierarchical order.

On this basis we propose an alternative *operative sequential iterative* algorithm. According to the character of their mutual interactions, the different processes are grouped into 'elementary blocks', so that each includes the minimum amount of information necessary for a complete description of its physical content. That is to say, each block constitutes an 'atomic problem', as it represents the minimum group of relations among the fundamental variables that can define a self-consistent physical problem. This set of elementary blocks is successively organized into a sequential structure that must be iterated in order to achieve the solution of the global problem.

Each block is processed independently: *(i)* the current values of the fundamental variables external to the block are taken as input data; *(ii)* the equations relevant to the block are then solved; *(iii)* the result yields as output the updated values of the fundamental variables internal to the block. It is a matter of experience that the iterations of such a procedure quickly converge to the physically correct solution, provided that the scheme has been properly tailored; i.e. if it is a faithful copy of the hierarchical structure of the interactions among the different physical processes. In this case the algorithm happens to be the analogical representation of the physics of the problem, as discussed in Section 8.3 of Paper I.

3. STRONG AND WEAK COUPLINGS

The intertwining of different physical processes and constraints brings about the coupling among different parts of the whole system. These couplings affect the links among the individual blocks of the numerical algorithm. Inside a stellar atmosphere, matter can be fairly considered to be in local thermodynamic equilibrium. On the other hand, the very existence of the emergent spectrum clearly shows that the radiation field departs from equilibrium. The common feature to all non-equilibrium situations is the appearance of long range coherence: macroscopically distinct parts of the physical system become correlated. This is in contrast to equilibrium situations where the range of correlations is determined by short-range interactions. In order to classify the different kinds of interactions that take place among the distinct components of our model, we may consider the range of action of the different processes considered. Short range interactions will individualize a sequence of regions, each governed by its local physics. On the other hand, long range interactions will imply the transfer of information among regions that are far apart by means of non-local transport processes. We may quite arbitrarily define the latter as a case of *strong coupling* and the former as *weak coupling*. From the mathematical point of view, different degrees of strength of the physical interactions are reflected in stronger or weaker ties among the fundamental variables of the model. These definitions will be sharpened in Section 6. Here we draw the reader's attention to the fact that the strength of the physical coupling between two components of a system has a correspondence, in the dual mathematical picture, in terms of the ease of exchange of information between them.

4. THE SYSTEM OF THE FUNDAMENTAL EQUATIONS

Let us rewrite the fundamental equations for a case more general than that discussed in Section 7.2 of Paper I. Here, we relax the simplifying hypothesis of hydrostatic equilibrium and allow for matter motions. The constitutive equations, namely the scalar equation of continuity and the vector Euler equation, then read

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \qquad (1)$$

and

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho (\mathbf{v} \cdot \nabla) \mathbf{v} = \rho \mathbf{g} - \nabla P, \qquad (2)$$

respectively.

The above set of four equations involves five fundamental variables, i.e. ρ, P, and the three components of $\mathbf{v}$. Further physical information is given by the equation of state,

$$P \;=\; \frac{k_{\mathrm{B}}}{m_{\mathrm{H}}\mu}\,\rho\,T\;, \qquad (3)$$

where k_{B} is the Boltzmann's constant, m_{H} the mass of the H atom, and μ the average mass of the particles. The equations are now five in number, but the unknowns have also grown in number, as the temperature T now makes its appearance.

In order to deal with the temperature, we have at our disposal the constraint of energy conservation, from which we derive the energy balance equation in which temperature plays a key role from the physical standpoint. Under the constraint of radiative equilibrium (RE), the energy balance equation reduces to

$$\int_0^\infty d\nu \oint d\mathbf{n}\;\left[\eta^{\mathrm{tot}}(\nu)\;-\;\chi(\nu)\,I(\mathbf{n},\nu)\right]\;=\;0\;. \quad (4)$$

The problem is that the radiation field appears explicitly in Eq. (4). We must therefore solve the system of RT equations that yield the values of the specific intensity necessary for the full description of the radiation field. Each specific RT equation, for a given $(\mathbf{n},\nu)$ pair, takes the form

$$\mathbf{n}\cdot\nabla I(\mathbf{n},\nu)\;=\;-\,\chi(\nu)I(\mathbf{n},\nu)\;+\;\eta^{\mathrm{tot}}(\nu)\;, \quad (5)$$

where $\eta^{\mathrm{tot}}(\nu)$ and $\chi(\nu) = a(\nu)+\sigma(\nu)$ are the macroscopic transport coefficients defined by Eqs. (27) and (28) of Paper I. In such a way we can eventually close the system of the fundamental equations.

If we introduce in the customary way the source function as

$$S(\nu)\;\equiv\;\frac{\eta^{\mathrm{tot}}(\nu)}{\chi(\nu)}\;, \qquad (6)$$

Eq. (5) can be rewritten in the form

$$\mathbf{n}\cdot\nabla I(\mathbf{n},\nu)\;=\;-\,\chi(\nu)\,\left[I(\mathbf{n},\nu)\;-\;S(\nu)\right]\;. \quad (7)$$

Once we define the branching parameter

$$\varepsilon_\nu\;\equiv\;\frac{a(\nu)}{a(\nu)\;+\;\sigma(\nu)}\;, \qquad (8)$$

we can recast the source function in the form

$$S(\nu,T)\;=\;\varepsilon_\nu\,B(\nu,T)\;+\;(1\;-\;\varepsilon_\nu)\,J(\nu) \qquad (9)$$

where $B(\nu,T)$ is the Planck function and

$$J(\nu)\;\equiv\;\frac{1}{4\pi}\oint I(\mathbf{n},\nu)\,d\mathbf{n} \qquad (10)$$

is the mean specific intensity. In this way we have expressed the source function as the sum of the thermal component $B(\nu,T)$ and the scattering term $J(\nu)$, weighted by the branching parameter ε_ν.

Furthermore, if we replace the generic geometrical variable x with the monochromatic optical deph τ_ν, defined by the differential relation

$$d\tau_\nu\;\equiv\;-\,\chi(\nu)\,dx\;, \qquad (11)$$

for the instance of plane–parallel geometry it holds that $\mathbf{n}\cdot\nabla = \mu\,d/dx$, where μ is the cosine of the angle formed by the direction $\mathbf{n}$ of propagation of the radiation beam and the outward normal to the plane–parallel layers. In this case Eq. (7) takes on the form

$$\mu\,\frac{dI(\mu,\nu)}{d\tau_\nu}\;=\;I(\mu,\nu)\;-\;S(\nu,T)\;. \quad (12)$$

From the mathematical point of view, the system of fundamental equations is heterogeneous. The constitutive equations link together local quantities. Eqs. (1) and (2) are differential equations, whose solution will be specified by the corresponding initial conditions. On the other hand, the energy balance equation involves the radiative flux, whose values are determined by solving the RT equations. The transport process links a non-local quantity (i.e. the radiative energy transported) with the source and sink terms of radiative transfer which are local quantities. Moreover, as mentioned in Section 7.2 of Paper I, the directional properties of radiative transfer put radiation beams into local contact, the corresponding RT equations having their initial conditions assigned at a different point in the stellar atmosphere. From the mathematical standpoint, we deal with a boundary condition problem.

5. ANALYSIS OF THE SEQUENTIAL APPROACH

According to the ideas discussed in Section 2, we must look for a proper sequence of elementary blocks that can lead to the numerical solution of the problem. Let us arrange the equations of Section 4 in the following order: Eq. (1) through Eq. (3), Eq. (5) and finally Eq. (4). This constitutes a sequence that follows what we might consider the natural order of the physical processes involved.

The sequence begins with the two constitutive equations. If we assume a trial estimate of the variable ρ (or alternatively $\mathbf{v}$), the equation of continuity will yield the corresponding values of $\mathbf{v}$ (or alternativey of ρ). Given ρ and $\mathbf{v}$, Euler's equation straightforwardly gives the pressure P. By means of the equation of state it is then possible to derive the temperature T. Hence, we have at hand all the ingredients necessary to compute the transport coefficients $\eta^{\mathrm{tot}}(\nu)$ and $\chi(\nu)$. From the successive solution of the RT equations we get the current values of the specific intensity of the radiation field.

At this point we can check whether the initial estimate of ρ (or $\mathbf{v}$) and the values obtained for $\mathbf{v}$ (or ρ), P, T, $\eta^{\mathrm{tot}}(\nu)$, $\chi(\nu)$, and the radiation field $I(\mathbf{n},\nu)$ satisfy the energy balance equation. In general, that will not be the case. We may, however, make use of

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Eq. (4) to compute the updated values of the bootstrap variable and repeat the cycle. One might expect that, through the run of successive iterations, the correcting procedure would eventually converge to a result that satisfies all the equations simultaneously. However, before undertaking the study of its convergence properties, one might enquire whether the above 'natural' sequence is indeed consistent with the physics of the problem.

A first classification of the properties of the stellar atmosphere physical system can be made by differentiating between *mechanical* (i.e. those corresponding to macroscopic motions) and *thermal* (i.e. relating to microscopic motions and the particles' internal structure) properties.

The constitutive equations determine the mechanical structure of the physical system; namely, they determine the relations among the variables ρ, $\mathbf{v}$, and P. They can therefore be grouped in a natural way into a *mechanical* block. Although linked with all the other variables, the former, however, play a prominent role inside the mechanical block. On the other hand, the transport equations and the constraint of energy conservation determine the internal energy and consequently shape the thermal structure of the physical system. Accordingly, they constitute the *energy* block. The coupling between the two blocks is brought about by the equations that describe the state of the matter in the stellar atmosphere, which, under the condition of thermal equilibrium (or at least of local thermal equilibrium), consist of the equation of state and the Boltzmann and Saha laws.

All these physical processes together shape the overall structure and govern the global behaviour of the stellar atmosphere physical system. By examination of Eqs. (1) through (5) it is easily seen that the thermal properties affect the mechanical behaviour by means of the equation of state which includes ρ, and the density ρ in turn affects the thermal structure as it enters Eq. (4) through the transport coefficients $\eta^{\text{tot}}(\nu)$ and $\chi(\nu)$.

The above physical analysis of the coupling among the different equations gives a straightforward answer to our previous question of whether it is physically sound to make use of the energy balance equation to correct the trial mechanical variable (either ρ or $\mathbf{v}$). If we want to keep the foregoing sequence of equations with the energy equation at the bottom as the corrector of the trial variable, it looks much more reasonable to choose the temperature as the variable to be corrected throughout the run of iterations because it is the protagonist inside the thermal block where the correction is performed. In such a way the original 'natural' sequence is confirmed on physical grounds, provided that the temperature T is chosen as the key variable of the whole procedure.

6. THE TEMPERATURE CORRECTION PROCEDURE

According to the foregoing statement of the problem, the computation of the structure of a stellar atmosphere is tantamount to the self-consistent determination of its temperature distribution, and the iterative sequential scheme under study corresponds to a temperature correction procedure. We are now going to undertake the study of its convergence properties. For the sake of economy, we neglect the true scattering of photons. This implies that $\sigma_\nu = 0$, hence $\varepsilon_\nu = 1$, and the source function $S(\nu, T)$ reduces to its thermal component $B(\nu, T)$. This assumption simplifies the mathematical development while retaining the essential difficulties of the physical problem.

6.1. The straight sequence procedure

Let us look back to the constitutive equations which allow us to eliminate the macroscopic velocity $\mathbf{v}$ and reduce Eqs. (1) and (2) to a single equation for ρ and P only, to be coupled with the macroscopic equation of state. In the latter, the information on the microscopic state of matter is contained in the function $\mu = \mu(\rho, T)$, which expresses the average molecular weight. Under conditions typical of stellar atmospheres, μ depends very little on the values of ρ and T. It always takes values between $1/2$ and $3/2$ so that it may be considered as constant to a first approximation. It must be stressed that, in the spirit of our sequential approach, the temperature is the external input data for the mechanical macroblock. Thus the block contains all the information necessary to define uniquely the mechanical structure in terms of the equations that describe the relevant physical processes, their initial conditions, and the external data which include the current trial value of the temperature. Because of the non-linear character of the above system, its solution requires a series of inner iterations whose result will be a set of current values for $\mathbf{v}$, ρ, and P that satisfy the equations of the mechanical macro-block consistently with the assumed initial value of T. These values will constitute part of the input for the next step, which consists of the solution of the RT and energy balance equations inside the energy macro-block.

The mechanical and the energy macro-blocks are coupled together through the transport coefficients. In order to get their values, which will complete the set of input data for the energy macroblock, we need the microscopic description of the stellar atmosphere material, which, under the conditions of the local thermodynamic equilibrium (LTE) is given by the laws of Boltzmann and Saha. (In the case that the LTE approximation does not hold valid, one must resort to the equations of statistical equilibrium.) As we neglect true scattering, inside the energy macro-block each specific RT equation is *independent* of all the others because each one has its own source function. Owing to the assumption that the current value T_0 of the temperature is an input data, all the source functions are known; that is, $S(\nu, T) = B(\nu, T_0)$. The solution of the RT system is then just the trivial solution of a set of independent first order linear ordinary differential equations. Once we have obtained the set of $I(\mathbf{n}, \nu)$ values solution of the system, we can straightforwardly compute the mean value of $J(\nu)$ values of the radiation field, hence the integral

$$J_a \equiv \int_0^\infty a(\nu)\, J(\nu)\, d\nu \; . \qquad (13)$$

We are now in a position to use the radiative equilibrium constraint, which we can rewrite as

$$\int_0^\infty a(\nu)\, J(\nu)\, d\nu \; = \; \int_0^\infty a(\nu)\, B(\nu, T)\, d\nu \; . \quad (14)$$

As the current value of J_a is known, the actual value T of the temperature can be straightforwardly obtained from Eq. (14), used as a trascendental equation. It must be stressed that under RE and LTE conditions the local temperature $T(r)$ is unambiguously determined by the single explicit law of conservation given by Eq. (14).

This sequence is then repeated with the updated value of the temperature. The flowchart of the sequential procedure is shown in Fig. 1.
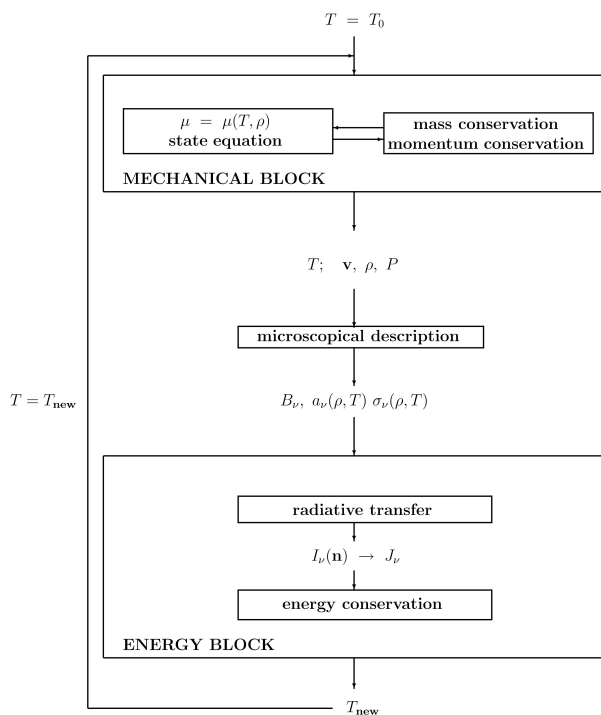
Fig. 1. *Flow-chart of the 'natural' sequential procedure.*

6.2. The Λ-iteration

It is a matter of fact, however, that the above strategy does not work when employed to compute a stellar atmosphere model. The series of successive temperature corrections tends to zero, but the rate of convergence is infinitely slow; even worse, the iterative procedure may converge to a solution that is spurious from the physical point of view. The question now is whether the method itself is globally incorrect, or whether the failure is due to specific localized drawbacks. Numerical experiments confirm that the inner iterative solution of the constitutive equations does work in practice. The cause of the failure has then to be sought inside the energy block, which we are going now to examine separately.

First of all, we examine the behaviour of the inner cycle of iterations shown in Fig. 2. This is a sequential scheme, akin to the general one outlined above: the RT equations are solved given the known current values of their source functions → the temperature is corrected by means of the energy conservation constraint → new source functions are computed.
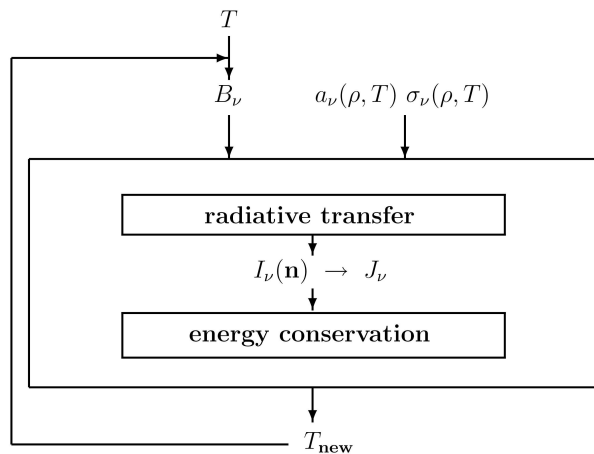
Fig. 2. *Sequential solution of the energy macro-block. The transport coefficients a_ν and σ_ν are input data defined outside the block. The input temperature, initially the trial input T_0, is the updated temperature $T = T_{new}$, the solution of the trascendental Eq. (14) at each iterative step. In the particular case here under consideration, it holds that $S_\nu = B_\nu$ and $\sigma_\nu = 0$.*

The above scheme is customarily called a Λ-iteration because the RT solution can be formally written in terms of the Λ-operator that appears in the solution of the Schwartzschild integral RT equation.[1] The Λ-iteration is an application of the Neumann series solution of linear integral equations of the second kind (Fredholm).[2] Application of the method to radiative transfer in stellar atmospheres nevertheless fails because of the large optical depth of the medium at many frequencies.[3] Radiative transfer, a non-local process, implies long range interactions among different parts of the atmosphere. In

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[1] For details see, for example, pp. 40–41 of Mihalas (1978).

[2] For a general discussion of this subject see, for example, Chapter III of Courant and Hilbert (1953). A brief summary can be found in Section 1.10.3 of Crivellari (2019).

[3] For a thorough discussion, see Section 6-1 of Mihalas (1978).

contrast, at each step of the Λ-iteration, the correction of the temperature is effective only within regions whose size is of the order of $\tau_\nu \sim 1$. The definition of strong coupling, given in Section 3, is justified by the above 'almost insuperable' difficulty brought about by the physics itself.

6.3. Simultaneous solution of the RT and RE equations

By solving sequentially the system of the RT equations and the RE condition, the foregoing iterative scheme has brutishly cut the Gordian knot of the physical coupling between radiative transfer and the constraint of radiative equilibrium. The violence done to the physics of the problem is repaid by the failure of the algorithm! The following discussion will shed light on the nature of this coupling.

In order to get rid of the above hindrance, one may consider the possibility of including the RE constraint directly in the source functions of the specific RT equations. If the Planck function is linearized around the current value T_0 of the temperature, namely

$$B(\nu, T) =$$

$$B(\nu, T_0) + \left[\frac{\partial B(\nu, T)}{\partial T} \right]_{T_0} (T - T_0) , \qquad (15)$$

to replace $B(\nu, T)$ in Eq. (14) by its expression given by Eq. (15) allows us to write

$$T - T_0 = \left(J_a - \int_0^\infty a(\nu) \, B(\nu, T_0) \, d\nu \right) /$$

$$\int_0^\infty a(\nu) \, [\partial B(\nu, T)/\partial T]_{T_0} \, d\nu . \qquad (16)$$

In this way the source function $S(\nu, T) = B(\nu, T)$, corresponding to the temperature that has to be determined consistently with the constraint of energy conservation, can be expressed in terms of quantities whose values are known and the term J_a that depends on the solution itself of the system of RT equations. That is to say, the set of independent RT equations. Eq. (12) transforms into the system of *coupled* equations

$$\mu \, \frac{dI(\mu, \nu)}{d\tau_\nu} = I(\mu, \nu) -$$

$$\left[f_1(\nu, T_0) - f_2(\nu, T_0) \int_0^\infty a(\nu) \, J(\nu) \, d\nu \right] . \quad (17)$$

The known functions f_1 and f_2 are evaluated from the current values of the input data of the energy macro-block. The solution achieved by solving the system of coupled equations Eq. (17) will yield a

set of $I(\mu, \nu)$ values consistent (but for the values of f_1 and f_2 that have been computed employing the current value T_0 of the temperature) with the RE condition. We shall thus be able to compute explicitly the term J_a from the values of the radiation field that correspond to the *temperature consistent with the energy constraint*.

Given this value of J_a, it is a trivial matter to render explicit the correct value of the temperature by solving the transcendental equation in T,

$$J_a = \int_0^\infty a(\nu) \, B(\nu, T) \, d\nu . \qquad (18)$$

The procedure, whose flow-chart is shown in Fig. 3, is then iterated until convergence is achieved.

However, this improved cycle of iterations does not work either. At the origin of the failure is the coupling of all the RT equations through the term J_a. From the mathematical standpoint this coupling transforms the solution of the system into a two-point boundary problem, because the incoming intensities have their initial conditions at the top, and the outgoing intensities at the bottom, of the plane–parallel atmosphere.
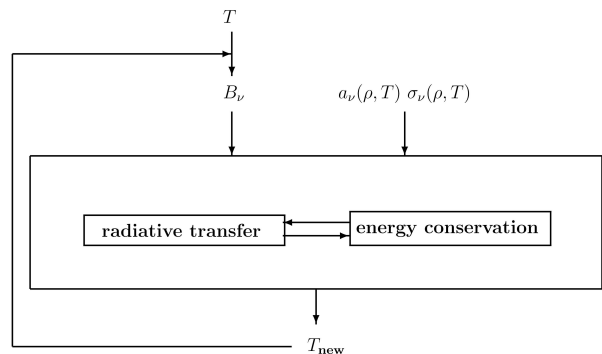
Fig. 3. *The energy macro-block: simultaneous solution of the RT and RE equations. The coupling between radiative transfer and the energy conservation constraint is brought about by the scattering-like integral J_a defined by Eq. (18).*

The difficulties intrinsic to the numerical solution of two-point boundary problems are well known. A solution by means of the method of discrete ordinates implies an eigenvalue problem of the order of the number of mesh points.[4] It may be possible to get rid of this severe drawback by employing implicit algorithms that allow one to express the solution at any given point as a function of the so far unknown solution at all the other points. The linearity of the elementary RT process makes that possible. However, the huge number of coupled equations renders the solution of the resulting linear system quite unmanageable by means of the customary discrete methods (e.g. Gauss-Seidel, Jacobi, etc.).

Such mathematical difficulties are the counterpart of the intrinsic nature of the physical problem.

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[4]For a discussion see Section 6-2 of Mihalas (1978).

The coupling term J_a, common to all the individual source functions of the specific RT equations, is the integral over all frequencies of the monochromatic mean intensity $J(\nu)$ weighted by the absorption coefficient $a(\nu)$. Although in the present case we neglect the true scattering of photons, the term J_a is formally similar to a scattering integral and brings about a fundamental difficulty, typical of any diffusion process: it carries information on the physical conditions of the atmosphere over a wide range of distances; the lower the opacity at a given frequency, the greater the distance. It turns out to be impossible in practice to solve a diffusion problem by means of an iterative procedure, which would essentially be akin to a Λ-iteration. The case under consideration here is a clear-cut example of that. The absorption coefficient $a(\nu)$ is characterized by step discontinuities and huge variations, sometimes of very many orders of magnitude. This implies great differences among the mean free path of the photons at different frequencies. Consequently, the physical information from points very far apart has to be carried by the radiative transfer process. On the other hand, for large values of the monochromatic optical depth τ_ν, $J(\nu)$ tends to $B(\nu, T)$. At a given depth within the atmosphere this effect is felt more by the more opaque frequencies whose contribution to the value of J_a is higher. An exceedingly large number of iterations would be necessary to achieve convergence. Even worse, the convergence could be to a physically wrong solution because the numerical precision of the computation will never be high enough to express the difference $J(\nu) - B(\nu, T)$ at each frequency point with a sufficient number of significant digits. Thus, physics accounts for the failure of the algorithm: the intrinsic strong coupling between radiative transfer and the RE contraint translates into a kink in the information pipeline at the corresponding point of the sequential algorithm. We show in the following section how it is possible to get rid of the above difficulty by softening the strong coupling by means of the Iteration Factors Method.

7. THE ITERATION FACTORS METHOD

The Iteration Factors Method (IFM) dates back to the generalization of the Variable Eddington Factors, originally introduced by E. Simonneau for the computation of LTE stellar atmosphere models in radiative equilibrium (Simonneau and Crivellari 1988), and later for the case where convective transport is also taken into account (Crivellari and Simonneau 1991). Fieldus et al. (1991) employed the method in their computation of a line-blanketed model atmosphere in spherical geometry. The IFM was applied to the line transfer problem in the paradigm case of a Two-Level-Atom by Simonneau and Atanacković-Vukmanović (1991) and Atanacković-Vukmanović (1991). The method was succesively generalized to the solution of the multilevel line transfer problem by Kuzmanovska-Barandovska and Atanacković (2010). Reviews of the IFM can be found in Atanacković-Vukmanović and Simonneau (1994) and in Section 3.7.3 of Atanacković (2019).

7.1. A new RT solution consistent with the RE constraint

Let us return to the RT equation in plane–parallel geometry, that is

$$\mu \frac{dI_\nu(x;\mu)}{dx} = -\chi_\nu(x) [I_\nu(x;\mu) - S_\nu(x)] , \quad (19)$$

where x is the geometrical path measured along the perpendicular to the layers. The zeroth and first order μ-moments of Eq. (19) are respectively

$$\frac{dH_\nu(x)}{dx} = -\chi_\nu(x) [J_\nu(x) - S_\nu(x)] \quad (20)$$

and

$$\frac{dK_\nu(x)}{dx} = -\chi_\nu(x) H_\nu(x) . \quad (21)$$

The first three μ-moments of the specific intensity $I_\nu(x;\mu)$ are, by definition,

$$J_\nu(x) \equiv \frac{1}{2} \int_{-1}^{1} I_\nu(x;\mu) d\mu , \quad (22)$$

$$H_\nu(x) \equiv \frac{1}{2} \int_{-1}^{1} I_\nu(x;\mu) \mu d\mu \quad (23)$$

and

$$K_\nu(x) \equiv \frac{1}{2} \int_{-1}^{1} I_\nu(x;\mu) \mu^2 d\mu . \quad (24)$$

We introduce now the Rosseland mean opacity $\chi_R(x)$ defined as

$$\frac{1}{\chi_R(x)} \equiv$$

$$\int_0^\infty \frac{1}{\chi_\nu(x)} \frac{\partial B_\nu[T(x)]}{\partial T} d\nu / \int_0^\infty \frac{\partial B_\nu[T(x)]}{\partial T} d\nu , \quad (25)$$

as well as the flux-weighted mean opacity

$$\chi_H(x) \equiv \int_0^\infty \chi_\nu(x) H_\nu(x) d\nu / \int_0^\infty H_\nu(x) d\nu =$$

$$\int_0^\infty \chi_\nu(x) H_\nu(x) d\nu / H(x) . \quad (26)$$

The change of the independent variable from the geometrical scale x to the Rosseland optical depth scale, defined by the differential relation

$$d\tau = d\tau_R \equiv -\chi_R(x) dx , \quad (27)$$

allows us to recast Eq. (20) in the form

$$\frac{dH_\nu(\tau)}{d\tau} = \frac{a_\nu(\tau)}{\chi_R(\tau)} [J_\nu(\tau) - B_\nu(\tau, T)] , \quad (28)$$

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where we have taken Eqs. (8) and (9) into account, and to rewrite Eq. (21) as

$$\frac{dK_\nu(\tau)}{d\tau} = \frac{\chi_\nu(\tau)}{\chi_R(\tau)} H_\nu(\tau) . \qquad (29)$$

By integration over the full frequency range, from Eqs. (28) and (29) we obtain the bolometric equations

$$\frac{dH(\tau)}{d\tau} = \frac{1}{\chi_R(\tau)} \times$$

$$\left[\int_0^\infty a_\nu(\tau) J_\nu(\tau) d\nu - \int_0^\infty a_\nu(\tau) B_\nu(\tau, T) d\nu \right] \quad (30)$$

and

$$\frac{dK(\tau)}{d\tau} = \frac{\chi_H(\tau)}{\chi_R(\tau)} H(\tau) . \qquad (31)$$

The RE constraint implies that the two integrals on the RHS of Eq. (30) must be equal so that $H(\tau)$ is constant, i.e.

$$H(\tau) = H = \frac{\sigma_{SB}}{4\pi} T_{eff}^4 , \qquad (32)$$

where σ_{SB} is the Stefan-Boltzmann constant and T_{eff} the effective temperature of the star. The constant value of H is a data of the problem that specifies the bolometric flux of the star. Eq. (31) then becomes

$$\frac{dK(\tau)}{d\tau} = \frac{\chi_H(\tau)}{\chi_R(\tau)} H . \qquad (33)$$

We now define the quantities

$$F(\tau) \equiv \frac{K(\tau)}{J(\tau)} \qquad (34)$$

and

$$\beta(\tau) \equiv \frac{\chi_H(\tau)}{\chi_R(\tau)} . \qquad (35)$$

Both are ratios between two homologous quantities: the former between the two first odd μ-moments of the specific intensity of the radiation field, and the latter between two mean opacities. The former, in particular, yields a closure relation for the system of the bolometric μ-moments. Thanks to the introduction of the two auxiliary functions $F(\tau)$ and $\beta(\tau)$, we can now rewrite Eq. (33) as a differential equation for the bolometric mean intensity $J(\tau)$, that is

$$\frac{d}{d\tau} [F(\tau) J(\tau)] = \beta(\tau) H . \qquad (36)$$

Eq. (36) is an RT equation for $J(\tau)$ that includes the RE constraint. That is to say, its solution simultaneously satisfies both the radiative transfer equations and the constraint of energy conservation. A convenient form for its initial condition is given by

$$J(\tau = 0) = \gamma H , \qquad (37)$$

which defines implicitly the quantity γ as the ratio

$$\gamma \equiv J(\tau = 0) \big/ H . \qquad (38)$$

If the functions $F(\tau)$ and $\beta(\tau)$ were known, as well as the value of γ, Eq. (36) could be straightforwardly integrated to yield the solution

$$J(\tau) = \frac{H}{F(\tau)} \left[\gamma F(\tau = 0) + \int_0^\tau \beta(t) dt \right] . \quad (39)$$

The bolometric mean intensity $J(\tau)$ obtained in such a way corresponds to a radiation field that automatically satisfies the RE constraint.

Let us define now the two average absorption coefficients

$$a_P(\tau) \equiv$$

$$\int_0^\infty a_\nu(\tau) B_\nu(\tau, T) d\nu \big/ \int_0^\infty B_\nu(\tau, T) d\nu \quad (40)$$

and

$$a_J(\tau) \equiv \int_0^\infty a_\nu(\tau) J_\nu(\tau) d\nu \big/ \int_0^\infty J_\nu(\tau) d\nu . \quad (41)$$

By means of a_P and a_J we can rewrite the RE constraint as

$$a_J(\tau) J(\tau) = a_P(\tau) B[T(\tau)] . \qquad (42)$$

The ratio

$$\alpha(\tau) \equiv \frac{a_J(\tau)}{a_P(\tau)} \qquad (43)$$

is again a homologous quantity which allows us to express the RE constraint as

$$B[T(\tau)] = \alpha(\tau) J(\tau) . \qquad (44)$$

According to the Stefan-Boltzmann law, $B[T(\tau)]$ is proportional to the fourth power of the temperature. Therefore, Eq. (44) yields an explicit formula to determine the temperature, consistent with the radiation field that simultaneously satisfies the RT and the RE equations. That is,

$$T(\tau) = \left[\frac{\sigma_{SB}}{\pi} \alpha(\tau) J(\tau) \right]^{1/4} . \qquad (45)$$

7.2. Iteration Factors

From the operational standpoint, the foregoing solution for $J(\tau)$ can be achieved only if the functions $F(\tau)$ and $\beta(\tau)$, as well as the initial condition γ, are known, which of course is not the case in the practice. In the example under consideration we are seeking the solution for the energy macro-block through an iterative procedure. The transport coefficients a_ν and σ_ν are given external data, hence $\beta(\tau)$ is known.

On the contrary, the ratio $K(\tau)/J(\tau)$ depends on the solution of the radiative transfer problem, which is an essential component of the energy block. We can, however, devise a new iterative scheme (see Fig. 4): a previous solution of the set of the independent monochromatic RT equations, where the specific source functions are computed with the old temperature, will yield the current values of $F(\tau)$ and γ. The approximate closure relation $F = K^{\text{old}}/J^{\text{old}}$ will allow us to solve Eq. (36) and consequently get the new temperature by means of Eq. (45). The source functions of the monochromatic RT equations can then be recomputed and a new closure relation obtained from the new RT solution.
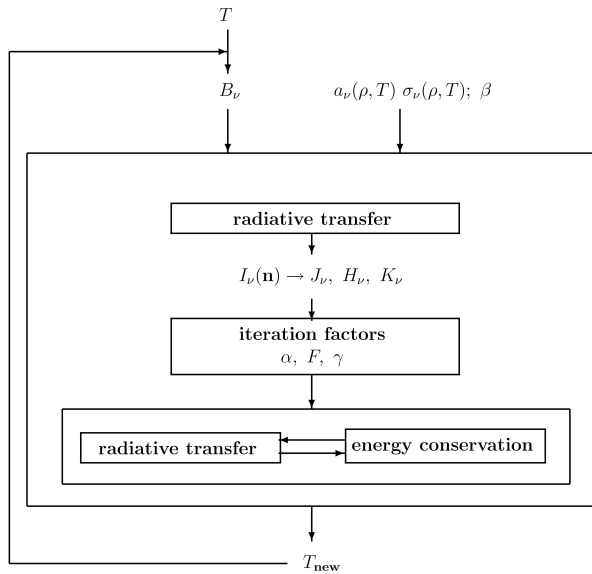
Fig. 4. *Iterative solution of the energy macro-block by means of the iteration factors. Here, the coupling between radiative transfer and energy conservation is brought about by the iteration factors β, F and γ. The latter are the carriers of information between the bolometric RT equation and the RE constraint.*

This new cycle of inner iterations for the energy macro-block quickly converges to the physically correct solution. The justification is quite straightforward. In the sequential solution of the energy macro-block (cf. Fig. 2) the 'radiative transfer' and 'energy conservation' blocks were coupled through the monochromatic mean values of the specific intensity. When the simultaneous solution of the RT equations and the RE constraint has been taken into account (cf. Fig. 3), the coupling is brought about by the scattering-like integral J_a defined by Eq. (13). In contrast, in the last scheme considered the 'energy conservation' block is replaced by a new one consisting of the solution of a bolometric RT equation consistent with the RE constraint. In the inner cycle of iterations inside the energy macro-block, information is carried from the 'monochromatic RT' block to the 'bolometric RT' block by means of the factors $F(\tau)$, $\beta(\tau)$, and γ. The physical coupling between the bolometric RT equation and the energy conservation constraint is brought about here by the above factors as it clearly results from the mathematical development presented in Section 7.1.

That marks the major difference to the previous case of the simultaneous solution of the monochromatic RT equations and the RE equation. Because they are the ratio of homologous quantities, factors like $\alpha(\tau)$, $\beta(\tau)$, $F(\tau)$, and γ are the optimum carriers of information from one block to another. Owing to their intrinsic nature, they 'filter' the error carried by the current values of the solution during the iterative correcting procedure. Although the latter can be far from the ultimate actual values, the ratio between homologous quantities mends possible off-set errors. These ratios therefore happen to be *quasi-invariant* during the iterative procedure and well deserve their name of Iteration Factors.

8. CONCLUSIONS

The foregoing study case, although a very specific one, is nevertheless an illustrative example of the strategy proposed for the numerical solution of the stellar atmosphere problem and allows us to draw some conclusions that hold valid for a wider class of problems. In the instance considered, as in most astrophysical problems, the RT equations are coupled through their corresponding source functions. The nature of this coupling is twofold. Firstly, the transport coefficients, and consequently the source functions, depend on the state of the stellar material, which in turn depends on the solution itself of the RT equations. This kind of coupling is non-linear and implicit. The straightforward sequential procedure, sketched in Fig. 1, might be envisaged in principle as the natural way to get rid of this difficulty. But we have seen in Section 6.2 that such an iterative scheme, equivalent to a Λ-iteration, does not work for the stellar atmosphere problem. The second kind of coupling is brought about by the scattering-like term J_a, which joins together the specific intensities $I(\mathbf{n}, \nu)$ corresponding to all directions $\mathbf{n}$ and frequencies ν. Eqs. (10) and (13) show that such a coupling is both linear and explicit. Consequently, from the mathematical point of view the solution of the system of the RT equations becomes a two-point boundary problem, as already stressed in Section 6.3. From the physical standpoint, the radiative transfer process carries information on the state of matter over a very wide range of distances, hence the failure of the iterative solution that includes the RE constraint in the source functions of the specific RT equations. In both cases the coupling between radiative transfer and the constraint of energy conservation turns out to be what we have defined as a strong coupling. The long range of the non-local transport process hinders the flow of information between the corresponding two blocks during the run of iterations for the solution of the energy macro-block. In contrast, for the reasons illustrated at the end of Section 7.2, to link the bolometric radiative transfer and the energy conservation blocks by means of the iteration factors β, F, and γ 'softens' the strength of the coupling.

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Because of their intrinsic nature as quasi-invariant quantities, the amount of spurious information carried by the iteration factors in successive steps of the iteration process is notably reduced. In terms of the solving algorithm, the easier flow of information reduces the originally strong coupling between the radiative transfer and the energy conservation blocks to a weak one. As a result, the rate of convergence of the iterative procedure based on the iteration factors is dramatically improved with respect to the previous schemes.

We conclude with a global remark. In order to design an operative procedure for the solution of a given problem, it is not possible to define general strategies: the physical nature of the specific problem considered must be taken into account case by case. Let us recall here H. Poincaré's words: *La physique ne nous donne pas seulement l'ocasion de résoudre des problemes ... Elle nous fait pressentir la solution.* Our achievement of a fast and reliable algorithm for the numerical solution of the stellar atmosphere problem is a good proof of that. The success of the iterative sequential procedure based on the iteration factors is the result of both putting into practice the principles discussed in Paper I and, above all, of the careful analysis of the physical problem performed in the present paper. On the basis of both common and our own experience, we would like to put forward the golden rule that it is the physics of the problem that dictates the operative algorithm for its solution.

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ЗВЕЗДАНА АТМОСФЕРА КАО ФИЗИЧКИ СИСТЕМ. II ОПЕРАТИВНИ СЕКВЕНЦИЈАЛНИ АЛГОРИТАМ ЗА РЕШАВАЊЕ ПРОБЛЕМА МОДЕЛОВАЊА ЗВЕЗДАНИХ АТМОСФЕРА

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У овом раду, који је други и последњи у серији, представљамо секвенцијални алгоритам за решавање проблема моделовања звезданих атмосфера који може служити као парадигма за решавање општијих нелинеарних и нелокалних проблема. Примењен је метод итерационих фактора (IF) за решавање једначина преноса зрачења заједно са условом равнотеже зрачења.