

ALTERNATIVE STRATEGIES TO SOLVE THE STELLAR ATMOSPHERE PROBLEM

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Abstract. At the heart of the computation of model atmospheres there is the so-called Stellar Atmosphere Problem, which consists of the self-consistent solution of the radiative transfer equations under specific constraints. The amazing progresses achieved in the field since the 1970s are due to both the dramatic increase of the computational facilities and the development of effective numerical algorithms. The purpose of this review is to draw attention to some methods, alternative to those that are mostly used nowadays such as the ALI methods. The improvement of the latter has been brought about by mathematical refinement, whereas the former are the result of a careful analysis of the physics of the problem. Rather than attempting an exhaustive presentation of these novel methods, which would be out of place here, the prime aim of this article is to sketch the main guidelines and to stress that it is always the physics itself that dictated the most effective algorithm.

1. INTRODUCTION

The comparison between observed and synthetic spectra is the key to the diagnostics of the physical and chemical properties of heavenly bodies. The computation of the spectral distribution of the electromagnetic radiation emitted by astrophysical objects requires the previous calculation of a model of their structure in terms of the fundamental dynamical and thermodynamic variables. This is tantamount to solve the Stellar Atmosphere Problem. As we will show, the latter is a non-local problem, owing to the transport of energy through the structure, and it is non-linear because of the coupling of all the relevant equations. To get rid of the second difficulty a straightforward approach would be to make the original system of equations linear and eventually convert it into a system of linear algebraical equations. Algorithms based on the Gauss-Seidel method can be envisaged for the numerical solution of the latter. In the practice of stellar atmosphere modelling several linearization methods have been introduced since the 1960s ¹.

¹For a basic review see Mihalas, 1978, Ch. 7. A recent general review on numerical methods in radiative transfer can be found in Atanacković, 2020, pp. 81-116.

Radiant energy is always transported in stellar atmospheres. The formal solution of the radiative transfer (RT) equation for the mean value of the specific intensity of the radiation field is given by the so-called Λ -operator. Numerical methods, based on the repeated application of the above operator (Λ -iteration methods) can be envisaged. However it is a matter of experience, justified by theoretical considerations, that the Λ -iteration is very slow (to say nothing that it may converge to a false solution). In order to speed up the convergence Accelerated Lambda Iteration (ALI) methods have been sought. Each element of the matrix representative the Λ -operator and its collocation has a precise physical meaning: it expresses the contribution to the radiation field, at a given point inside the stellar atmosphere, originating at distant points (non-local aspect of RT). The greater the optical path from the point source, the more removed from the diagonal of the matrix is the corresponding element. By taking this into account, ALI methods replace the original full matrix used in the straightforward Λ -iteration with an approximate diagonal (or n -diagonal) matrix. From the mathematical point of view ALI is the application of preconditioning to the iterative solution of a linear system of equations². A review of ALI methods can be found in *Stellar Atmospheres: Beyond Classical Models* (Crivellari et al. 1991).

The improved rate of convergence brought about by ALI methods is due to mathematical improvements. In contrast, we present here alternative sequential methods, which have been designed taking into account the physics that governs the structure of a stellar atmosphere. After mentioning the algorithmic representation of physical systems in Sec. 2, we list the fundamental equations of the stellar atmosphere problem in Sec. 3. Successively in Sec. 4 we show the way they are solved sequentially within an iterative procedure, whose effectiveness is brought about by the use of iteration factors that we are going to discuss in some detail in Sec. 5. The seminal idea introduced by Eduardo Simonneau (Simonneau and Crivellari, 1988; Simonneau and Atanacković-Vukmanović, 1991) has been developed and applied by Olga Atanacković and coworkers to several line transfer problems. Their main results are presented in Sec. 5. Future applications of the foregoing strategy to the modelling of the circumstellar envelopes of AGB stars will be mentioned in Sec. 6.

2. ALGORITHMIC REPRESENTATION OF PHYSICAL SYSTEMS

This is not the place for a philosophical inquiry into the reality of the phenomenological world. All that we want here is to achieve an effective description of physical systems; in other words a representation of their structure³. As a necessary premise let us first introduce two definitions:

- (i) By physical system we mean any arbitrary set of objects that can be identified and quantified by means of physical variables. To specify the state of the system a proper set of variables must be chosen that is necessary and sufficient to include the maximum available information required to determine both the properties of the system at a given time and its future evolution.
- (ii) We define the structure of a system as the organization of the parts into which it can be ideally separated. The structure shall be shaped by the mutual interactions among these components.

²See Atanacković, 2020, p. 112.

³For more details see Crivellari (2005).

Following Bridgman's operational perspective ⁴ we ideally dissect a physical system into an ensemble of simpler interacting parts so that we can describe the global behaviour of the system in terms of the laws governing its elementary components. Such a process leads eventually to a *model* of the physical system that, for its own analytical nature, can be easily translated into set of equations that constitute a *mathematical model*. The exact solution of this system of equations is not possible in general. The unavoidable numerical solution can be achieved via discretization; for instance, by means of a discrete ordinates method. After that the original system of equations has been replaced by the corresponding system of discrete equations, it is matter to seek for a suitable numerical algorithm for their solution.

If each stage of the previous steps has been worked out properly, the structure of the ultimate *algorithmic model* will be akin to that of the original model. It may therefore be considered as an operative representation of the physical system under study. Joseph Fourier claimed that the relations among the mathematical functions of the physical variables and their derivatives are not just matter of calculus; they are actually present in the natural phenomena themselves ⁵. According to this point of view the general scheme, required to convert the mathematical model into numerical information by means of algorithms, partakes of Nature, too. This somewhat naive form of realism, together with Henri Poincaré's statement ⁶ that "*La physique ne nous donne pas seulement l'ocasión de résoudre des problèmes ... Elle nous fait sentir la solution.*" shall be our tenet in the quest for the optimum algorithm.

3. THE FUNDAMENTAL EQUATIONS OF THE STELLAR ATMOSPHERE PROBLEM

We will go beyond Auer's definition (Auer, 1971) and say that the *Stellar Atmosphere Problem* consists in the solution of the equations that define the structure of a stellar atmosphere under specific assumptions, i.e. constraints, initial and boundary conditions, simplifying hypotheses.

3. 1. THE EQUATIONS

The fundamental equations are listed in Table 1. From the macroscopic standpoint the constitutive equations link the variables P, ρ and \mathbf{v} that shape the fluid dynamic structure. They play a protagonist role in what we call the *mechanical block*. With regard to the energetics of the system, the transport and energy equations determine its internal energy and hence the thermal structure. They constitute our *energy block*, whose protagonist variable is the temperature T .

The foregoing equations are the continuous mathematical representation of the physics that shapes the structure of a stellar atmosphere, described by the values adopted at each point by the fundamental physical variables. These values are determined by:

⁴P.W. Bridgman (1882 - 1961) American physicist, Nobel Prize for Physics in 1947. In order to get rid of the ambiguities inherent in the definition of scientific ideas, he introduced an 'operational' approach to scientific meaning, described in his book *The Logic of Modern Physics* (1927). Operationalism consists in defining physical concepts in terms of the operations, both physical and mental, involved in their measurement.

⁵J.-B. J. Fourier: 1831, *Analyse des Équations Déterminées*, (Paris: Firmin Didot frères), p. 185.

⁶H. Poincaré: 1911, *La valeur de la Science*, (Paris: Flammarion), Ch. V, p. 153.

Table 1: The fundamental equations that shape the structure of a stellar atmosphere.

| | |
|--------------------------------------|---|
| Constitutive equations: | conservation of mass and momentum equation of motion |
| Equation of state: | macroscopic LTE state of matter |
| Microscopical description of matter: | atomic occupation numbers: Boltzmann and Saha laws in LTE statistical equilibrium equations in non-LTE |
| Transport equations: | radiative transfer convective transport |
| Energy equations: | conservation of energy both for matter and the radiation field |

- the relations among the variables;
- the constraints imposed by the external conditions;
- the internal energy of the system.

3. 2. A NON-LINEAR AND NON-LOCAL PROBLEM

The essential difficulty of the stellar atmosphere problem arises because all the physical variables interact throughout the whole atmosphere. The problem is therefore strongly *non-linear*. Moreover, the local variation of a variable can have an important effect on the properties at a great distance, giving rise to a *non-local* problem. In principle it could be possible to overcome the former drawback via a proper linearization technique that convert the original system of equations into the equivalent system of linear algebraical equations, but in the practice such a direct approach is often unfeasible. In the specific case of the stellar atmosphere problem the number of discrete points that warrant an adequate coverage for the behaviour with depth of the structure, as well as that required to cover the range of frequencies for radiative transfer, turns out to be exceedingly high. The dimensions of the matrix of the coefficients of the system may be therefore as large as 10^4 . It is well known that the numerical inversion of large or ill-conditioned matrices is a severe problem. In a seminal paper on the numerical inversion of matrices of high order von Neumann and Goldstine (1947) consider that, in order to be suitable for numerical computation, transcendental operations and implicit definitions (e.g. the solution of algebraical equations) must be replaced by algorithms involving only those elementary operations that computers can handle directly. Consequently, they state that, when 'exact' (transcendental) arithmetic is replaced by 'approximate' arithmetic, no computing machine can perform all the operations faultlessly because of the finite number of digits available.

4. ITERATIVE SOLUTIONS OF THE STELLAR ATMOSPHERE PROBLEM

Since the 1960's a lot of iterative algorithms have been conceived in order to achieve the numerical solution of the Stellar Atmosphere Problem. In the following we are going to compare the widely used Complete Linearization Method with our own sequential approach, firstly devised by Eduardo Simonneau in the 1980's.

4. 1. COMPLETE LINEARIZATION METHOD VS. ITERATIVE SEQUENTIAL APPROACH

The basic idea of the *Complete Linearization Method* (CLM) ⁷ is to write the system of fundamental equations in terms of a starting approximate solution and to expand linearly the relevant variables around the values given by the former (linear perturbation). By replacing the original variables with their linear expansion one obtains a system of linear algebraical equations in which the new unknowns are the perturbations of the variables. This scheme is then iterated to convergence. At the basis of the CLM is the assumption, explicitly stated by Mihalas, that no one variable is more 'fundamental' than any other, for they all interact mutually.

Against such an 'egalitarian' treatment we shall remark that: (i) the different processes are characterized by very different scales; (ii) the strength of the coupling among the different phenomena may vary considerably case by case. A *sequential* procedure may therefore be envisaged. According to the nature of their mutual interactions, we individualize the different processes and group them into *elementary blocks* such that each of the latter contains the statement of a *self-consistent* physical problem. We may define these problems as 'atomic', in the sense that the relevant physical information cannot be further reduced. Afterwards the elementary blocks are organized into a sequence in which the atomic problems are solved one by one. Data coming from the solution of upstream blocks are of course required for the solution of the one under consideration, which will constitute the input for the downstream blocks. At the core of an effective strategy to solve the global problem is finding the proper sequence of the elementary blocks.

The equations in Table 1 are listed according to a certain order that may be considered as 'natural'. The mechanical block, which includes the constitutive equations together with the equation of state, accounts for the dynamic and thermodynamic properties of the stellar atmosphere material. It is therefore the first to be solved. However, the number of available equations is less than that of the variables involved; in the most general case 5 equations for the 3 variables T, P, ρ and the 3 components of the vector \mathbf{v} . The amount of energy carried on throughout the atmosphere (mainly by radiative transfer) under the constraint of energy conservation is considered in the energy block, whose protagonist variable is T , as already mentioned. The coupling of the two blocks via the microscopic description of matter allows the closure of the global system of equations.

Of course, the solution of the foregoing system requires a numerical algorithm. The above considerations dictate in a natural way the *sequential* approach, sketched in Fig. 1. If an initial guess of the run of one of the fundamental variables is given, the number of the variables is equal to that of the equations of the mechanical block, which therefore can be solved. The microscopic state of matter can then be determined,

⁷See Mihalas, 1978, pp. 230-234.

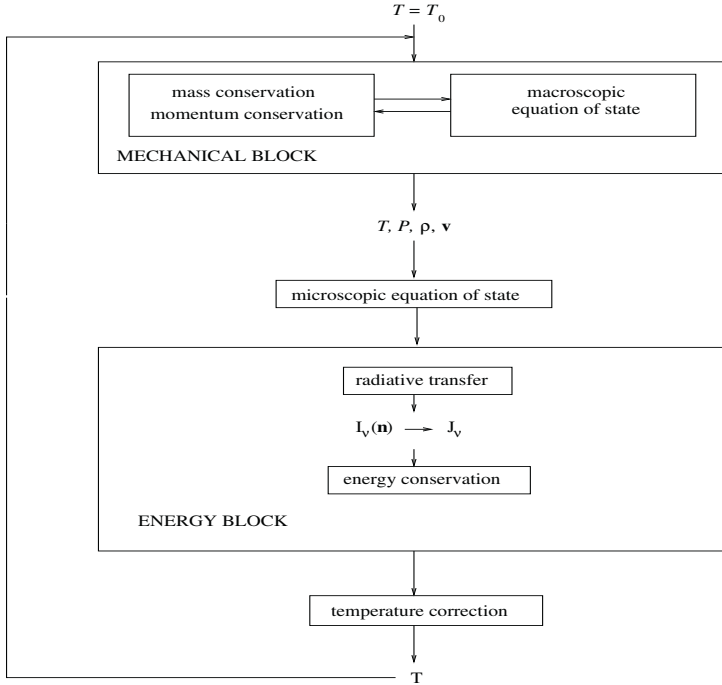


Figure 1: The 'natural' sequential procedure. In the mechanical block the constitutive equations are solved simultaneously. The correction of the current temperature distribution is achieved after the energy block. For an atmosphere in radiative equilibrium the RE constraint can be used as a transcendental equation to correct the current temperature T . Such an iterative procedure is equivalent to a Λ -iteration.

so that the emissivity η_ν and extinction $\chi_\nu = a_\nu + \sigma_\nu$ (the macroscopic transport coefficients that define the RT equations) can be computed. The solution of the system constituted by the latter yields the values of the specific intensity of the radiation field, $I_\nu(\mathbf{n})$, and its mean value J_ν . At this point the constraint of energy conservation can be checked. In general it will be not satisfied and the run of the trial variable has to be up-dated. Because the constraint of energy conservation involves the internal energy $U(T)$, T is the logical choice for the trial variable. In particular, when the simplifying hypothesis of radiative equilibrium (RE) is assumed, the corresponding energy conservation equation can be used as a transcendental equation in T to correct the current trial distribution. Then the sequential scheme is iterated until a prefixed criterion of convergence is achieved.

It is, however, a matter of experience that the foregoing 'natural' scheme does not work in the practice. The iterative solution of the coupled equations in the mechanical block is quickly obtained. But the convergence of the global procedure, namely the successive corrections of the temperature, is either infinitely slow or may even converge to a solution, which is false from the physical standpoint. This should be expected because the iterative solution inside the energy block is akin to a Λ -iteration, whose drawbacks are well known.

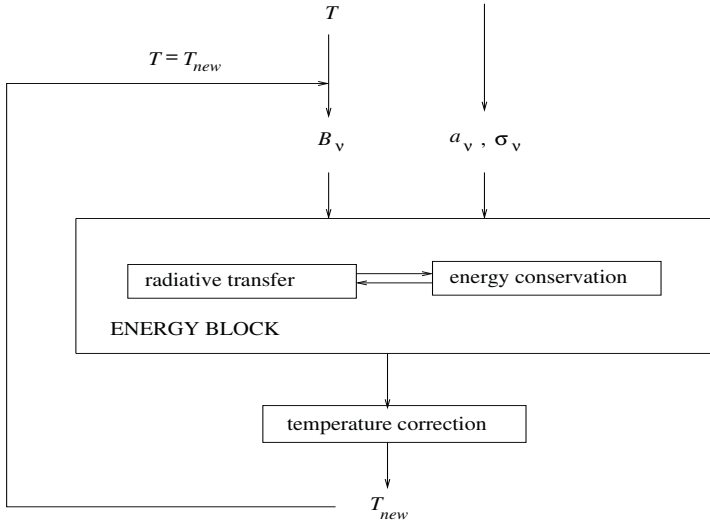


Figure 2: Simultaneous solution of radiative transfer and the RE constraint. The latter is included in the source function of each specific RT equation.

4. 2. COUPLING OF THE RT AND ENERGY CONSERVATION EQUATIONS

The sequential procedure in the energy block can be replaced by the simultaneous solution of the coupled RT and energy conservation, like the constitutive equations in the mechanical block (see Fig. 2.) For the sake of an illustrative example let us consider a stellar atmosphere in radiative equilibrium. In this case, taking into account the customary form of the source function $S_\nu = \varepsilon_\nu B_\nu + (1 - \varepsilon_\nu) J_\nu$, where $\varepsilon_\nu \equiv a_\nu / (a_\nu + \sigma_\nu)$, the equation of energy conservation reduces to

$$J_a \equiv \int_0^\infty a_\nu J_\nu d\nu = \int_0^\infty a_\nu B_\nu(T) d\nu, \quad (1)$$

where J_a accounts for the amount of radiant energy absorbed and $B_\nu(T)$ is the Planck function. We can linearize the latter around the value $B_\nu(T_0)$ corresponding to the trial temperature distribution, that is

$$B_\nu(T) = B_\nu(T_0) + \left(\frac{\partial B_\nu}{\partial T} \right)_0 (T - T_0). \quad (2)$$

By taking into account eqs. 1 and 2 it follows that the correction of the temperature can be expressed as

$$T - T_0 = \left[J_a - \int_0^\infty a_\nu B_\nu(T_0) d\nu \right] / \int_0^\infty a_\nu \left(\frac{\partial B_\nu}{\partial T} \right)_0 d\nu. \quad (3)$$

Consequently, we can rewrite eq. 2 as

$$B_\nu(T) = f_1(\nu; T_0) + f_2(\nu; T_0) J_a , \quad (4)$$

where the values of f_1 and f_2 are computed with the trial value T_0 of the temperature. By substitution, the source function can be written as

$$S_\nu = \varepsilon_\nu [f_1(\nu; T_0) + f_2(\nu; T_0) J_a] + (1 - \varepsilon_\nu) J_\nu . \quad (5)$$

Recast into this form the source function of each specific RT equation includes the RE constraint. All the specific equations are coupled through the common term $J_a \equiv \int a_\nu J_\nu d\nu$. The problem is that this integral is formally akin to a diffusion integral. To solve iteratively a diffusion problem is equivalent in the practice to a Λ -iteration. The intrinsic difficulty arises from the coupling in the source function of each RT equation of all the monochromatic specific intensities, that is to say *all the individual solutions*, which are characterized by different height scales due to the huge difference of opacity with frequency. Ostensively we can define the above one, brought about by the long-range interactions, as a *strong* coupling. In contrast the rapid iterative simultaneous solution of the equations of the mechanical block justifies labelling their coupling as *weak*.

5. THE ITERATION FACTORS METHOD

A smart strategy to soften the strong coupling between the RT equations and the RE constraint has been conceived by Eduardo Simonneau. Such an approach, the *Iteration Factors Method*, fully generalizes the idea of the Variable Eddington Factors (VEF)⁸. A first application to the iterative temperature correction in a stellar atmosphere (Simonneau and Crivellari, 1988) was succesively used for the computation of stellar atmosphere models when convective transport is taken into consideration (Crivellari and Simonneau, 1991),

5. 1. FUNDAMENTALS OF THE METHOD

As an illustrative example, we consider the particular but paradigmatic case of a plane-parallel stellar atmosphere in radiative equilibrium. The first two μ -moments of the relevant RT equations integrated over the full frequency range (bolometric) that link the bolometric μ -moments J , H and K of the specific intensity of the radiation field, are

$$\frac{dH(\tau)}{d\tau} = \frac{1}{\chi_R(\tau)} \left[\int_0^\infty a_\nu J_\nu d\nu - \int_0^\infty a_\nu B_\nu(T) d\nu \right] \quad (6)$$

and

$$\frac{dK(\tau)}{d\tau} = \frac{\chi_H(\tau)}{\chi_R(\tau)} H(\tau) , \quad (7)$$

where τ and χ_R are the Rosseland optical depth and mean opacity, respectively, and

⁸See Mihalas, 1978, pp. 46-47.

$$\chi_H(\tau) \equiv \int_0^\infty \chi_\nu(\tau) H_\nu(\tau) d\nu / H(\tau) . \quad (8)$$

In eq. 8, $\chi_\nu = a_\nu + \sigma_\nu$ is the monochromatic extinction (i.e. absorption plus scattering) coefficient. The RE constraint requires the two integrals on the RHS of eq. 6 to be equal; it holds, therefore, that $H(\tau) = H = \text{const}$. The constant H is fixed by the luminosity of the star and is a *datum* of the problem. If we define now

$$\beta(\tau) \equiv \chi_H(\tau) / \chi_R(\tau) , \quad (9)$$

we can rewrite eq. 7 as

$$\frac{dK(\tau)}{d\tau} = \beta(\tau) H . \quad (10)$$

The further definition of a ratio akin to the VEF, that is

$$F(\tau) \equiv K(\tau) / J(\tau) , \quad (11)$$

will yield the necessary closure for the system constituted by the first two μ -moments of the bolometric RT equation. Thanks to the above factor we can recast eq. 10 in the form

$$\frac{d}{d\tau} [F(\tau) J(\tau)] = \beta(\tau) H . \quad (12)$$

This is an RT equation for the bolometric mean specific intensity that *includes the RE constraint*.

By introducing the customary definition of the absorption mean $a_J \equiv \int a_\nu J_\nu d\nu / J$ and the Planck mean $a_P \equiv \int a_\nu B_\nu(T) d\nu / B(T)$, after defining the factor

$$\alpha(\tau) \equiv a_J(\tau) / a_P(\tau) \quad (13)$$

we can rewrite the RE constraint as

$$B(T) = \alpha(\tau) J(\tau) . \quad (14)$$

If $J(\tau)$ is known, eq. 14 gives the 'corrector' of the current temperature and the new temperature, *consistent with the RE constraint* will be

$$T(\tau) = \left[\frac{\pi}{\sigma_{rad}} \alpha(\tau) J(\tau) \right]^{1/4} , \quad (15)$$

where σ_{rad} is the Stefan-Boltzmann constant.

5. 2. ITERATION FACTORS FOR THE SOLUTION OF THE ENERGY BLOCK

The solution for $J(\tau)$ consistent with the RE constraint, as given by eq. 12, is obtained only if $\beta(\tau)$ and $F(\tau)$ are known. When dealing with the energy block in the course of the iterative sequential procedure the transport coefficients a_ν and σ_ν are external data, hence $\beta(\tau)$ is given. On the contrary, the ratio $F(\tau) = K(\tau)/J(\tau)$ depends on the previous solution of the RT equations. An operative solution can be achieved by means of a new iterative scheme inside the energy block. The first

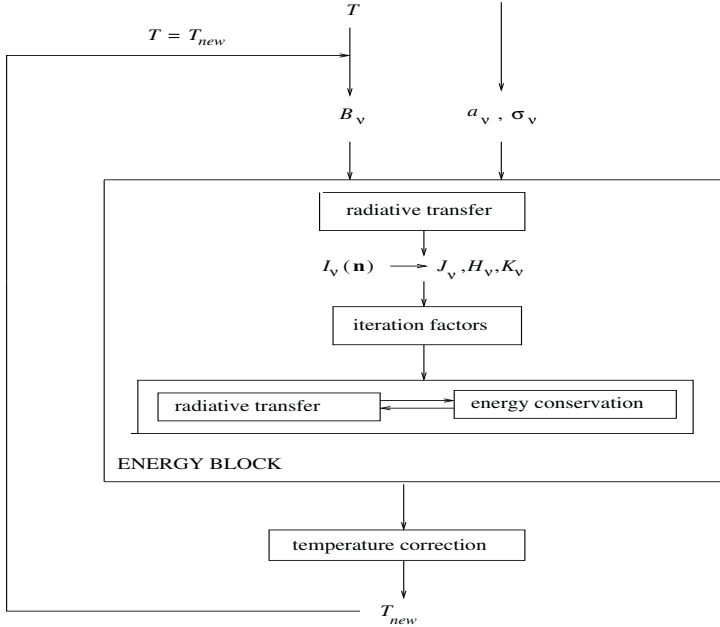


Figure 3: Simultaneous solution of the RT equation for J and the RE constraint obtained introducing proper iteration factors that convert the coupling into a 'weak' one.

step consists in the solution of the specific RT equations, whose source functions are computed with the current temperature distribution and the transport coefficients (the input to the block). The approximate closure for the system of the μ -moments of the bolometric RT equations, that is $F(\tau)$, can then be computed in order to solve eq. 12. On the other hand the factor $\alpha(\tau)$, the key to correcting the temperature via eq. 15, is computed from the values of J_ν , the solution of the specific RT equations. This scheme (see Fig. 3) is iterated with the up-to-dated temperature until a given convergence criterion is satisfied.

Experience shows that this new procedure rapidly converges to a solution that is correct from the physical standpoint, owing to the fundamental fact that the coupling between the RT equation for $J(\tau)$ and the RE constraint is now brought about by the ratio $K(\tau)/J(\tau)$ and not by the integral $J_a \equiv \int a_\nu J_\nu d\nu$, as in the previous scheme for the energy block. The foregoing *strong* coupling has been converted into a *weak* one. The success of the above strategy is essentially due to the introduction of the factors $\alpha(\tau)$, $\beta(\tau)$ and $F(\tau)$. Because of their intrinsic nature they carry on information optimally from a block to the successive one. As they are a ratio between homogeneous quantities, they mend the errors that affect the current values by eliminating wrong factors of scale. We call such ratios, that prove to be good *quasi-invariants* along the iterative sequential procedure, *Iteration Factors*.

5. 3. DEVELOPMENTS AND FURTHER APPLICATIONS

The convergence of some of the iterative methods currently in use can be greatly accelerated when we treat separately, within a *forth-and-back process*, the natural two-stream representation of the radiation field along each line of propagation. Integral methods based on the Λ -operator employ an *implicit* representation of the source function when computing the mean intensity of the radiation field. In contrast to the above scheme, which might be regarded as *global*, one may consider a *local* implicit scheme: the specific intensity propagating along a given direction is expressed at a given point as a linear combination of the unknown values of the source function S and its first derivative S' at that point. In contrast with other ALI methods, the FBILI method proposed here is a two-point algorithm that works by taking into account the values of S and S' on pairs of successive depth points. In the first step of an iterative procedure, the *forward-elimination* (FE), the values of the incoming specific intensities, as well as the coefficients of the linear relation above mentioned, are computed with the formal solution of the RT equation by using the known current values of S and S' . These coefficients are stored to be used in the successive *back-substitution* (BS). The FE starts at one of the end points, where the given value of the incoming specific intensity sets one of the boundary conditions, and sweeps inwards all the inner points up to the last one, where the outgoing specific intensity is given by the second boundary condition. In the BS the up-dated values of the source function are computed together with those of the outgoing intensities.

Such a simple and efficient approach, called as *Forth-and-Back Implicit Λ -Iteration* (FBILI), has been introduced by Atanacković-Vukmanović (1991) and later developed by Atanacković-Vukmanović et al. (1997). The implicit representation of the source function in the computation of the intensities within the above iterative scheme dramatically accelerates the rate of convergence of the iterative process while retaining the straightforwardness of an ordinary Λ -iteration. This is mainly because, in the FE when the coefficients of the implicit linear relation are computed, the only piece of information that the FBILI retains from the previous iteration at each depth point is the value of a single *iteration factor*, i.e. the ratio of the non-local part of the ingoing mean intensity to that of the current source function S_0 . This iteration factor is used in the next step of iteration. It is worth stressing that the implementation of this new method comes from physical considerations, not from a previous analysis of the mathematical properties of the problem. Once again it is physics that dictates the optimum algorithm.

Along the foregoing guidelines, significant developments and new applications to the line formation problem have been introduced by Olga Atanacković and coworkers at the Faculty of Mathematics of the University of Belgrade. Let us quote here only the most significant results. *The Iteration Factors Method for the line formation problem*: for the paradigm problem of the Two-Level Atom line transfer Atanacković-Vukmanović (1991), Atanacković-Vukmanović and Simonneau (1994); for multi-level atom line transfer Kuzmanovska-Brandovska and Atanacković (2010). *The FBILI method for multi-level line transfer*: Kuzmanovska, Atanacković and Faurobert (2017). *The FBILI method for radiative transfer in 2D*: Milić and Atanacković (2014).

6. MODELLING AGB STARS AND THEIR CIRCUMSTELLAR ENVELOPES

Sergio Cristallo and Luciano Piersanti at the INAF - Oss. Astronomico d'Abruzzo (Italy) are conducting a research project to study giant stars on the asymptotic branch of the Hertzsprung-Russell diagram (AGB stars) and their circumstellar envelopes; it is part of the n_TOF (neutron time-of-flight) experiment at CERN. In particular, they concentrate on circumstellar envelopes. Besides the modelling of the overall structure and atmosphere of AGB stars, the subjects covered include the formation of molecules and dust grains in their neighborhood. The complex interactions among the physical processes involved require effective *ad hoc* numerical methods for the solution of the relevant non-local and non-linear problem. A first step into this direction has been the construction of the hydrodynamic code VULCAN that can follow the propagation of shocks in the circumstellar envelopes of AGB stars (Cristallo et al. in preparation). Modelling AGB stars implies to take into consideration the physical properties of both their outermost layers and the circumstellar medium, as well as the hydrodynamics of the material lost during the stellar lifetime, all of which requires proper solutions for the constitutive equations, the equation of state and the RT equations. The architecture of the Iterative Sequential Approach allows for direct control over the results of each elementary block and their quantitative effects on the structure of the atmosphere brought about by each physical process. Therefore, to adopt this strategy will greatly help the implementation of the corresponding numerical algorithms in the VULCAN code. Preliminary results have been achieved. A test model atmosphere has been computed under the simplifying hypotheses of hydrostatic and radiative equilibrium. The significant improvements introduced are: (i) the previous solution of the 1D RT has been replaced by the 3D solution obtained with the Implicit Integral Method of Simonneau and Crivellari (Simonneau and Crivellari, 1993; Gros et al., 1997) ; (ii) after the due revision of the equation of state to take into account the H₂ molecule and compute the corresponding atomic population, the contributions of selected molecules (CO, H₂O, SiO and TiO) have been included in the opacity of the stellar material; (iii) the injection of non-radiative energy in the outer layer, in order to mimic the passage of a shock, has been considered. The next steps will be the removal of the current simplifying hypothesis of hydrostatic equilibrium to allow for the correct fluid dynamics treatment, as well as the inclusion of convective transport.

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This article is dedicated to my mentor and friend Eduardo Simonneau, who conceived the ideas at the basis of the algorithms and methods presented here and had a substantial part in their implementation. I am happy to thank the organizers of the XIX Serbian Astronomical Conference, and my friend Olga in particular, for the opportunity to review our longstanding collaboration and to outline future applications.

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