A numerical laboratory for the diagnostics of stellar properties

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Abstract. In a recent paper (Crivellari et al., 2003) we summarized the principles of the algorithmic representation of the structure of a stellar atmosphere. We mentioned there our recent progresses in the numerical treatment of both the global method and the basic components of the corresponding models. As the natural sequel to that paper, we wish to outline here the iterative sequential procedure that we have designed for the computation of such models, and briefly comment about the possibilities that it offers.

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1. A numerical laboratory

The intrinsic difficulty of the numerical solution of the stellar atmosphere problem arises from its non-local and non-linear character: each variable of the problem interacts with all the others at every point of the atmosphere due to the presence of the radiative transfer process. The solutions currently in use are based on a linearization of the non-linear terms, and eventually requires the solution of a huge system of linear algebraical equations. But such a "brute force" approach involves not only a high risk of destructive numerical instabilities, but also the possibility of obtaining solutions spurious from the physical point of view.

In alternative we have developed a novel sequential iterative scheme, designed in agreement with the physical nature of the problem. According to our experience, an iterative procedure quickly converges to the physically correct solution, provided that the scheme reflect the hierarchical structure of the iterations among the different processes. (For details, see Crivellari 2002.)

Our method does not require any matrix computation because it solves sequentially a series of elementary problems.

The simple structure of the whole algorithm permits a direct control onto the
partial results obtained in each of its parts, and allows us to treat each one of them with the required numerical accuracy, according to the relevant physical properties.

Thus we have now at hands an unparalleled benchmark to ascertain the quantitative effects on the structure of the atmosphere (and by the way on the diagnostics of the stellar properties) brought about by each one of the intervening specific physical processes: we can make experiments through numerical computation.

2. The iterative correction procedure

The distinctive feature of the algorithm comes from its organization into macroblocks. Within each of them a self-consistent physical problem is solved by assuming that the current values of some input variables are known, so that the updated values of the output variables of the block can be obtained. Such a treatment constitutes a numerical simulation of the physical processes that are at their origin of the corresponding equations.

In Fig. 1 we show the flowchart of our procedure. We consider here the paradigm case of a model atmosphere under the simplifying hypotheses of hydrostatic and local thermodynamical equilibrium. For sake of economy, inside the energetic macroblock we show only the computation of the radiative flux and the corresponding radiative temperature correction. Actually also the convective flux is computed in the program, together with the corresponding convective temperature correction.

The block-diagram of our sequential iterative procedure contains two macroblocks: the structural and the energetic one, coupled through the equation of state.

2.1. The structural macroblock

The input of each step of iterations is the temperature $T_i(r)$, whose values stay constant inside the structural macroblock. The latter consists of two coupled blocks. The first one accounts for the condition of hydrostatic equilibrium; the second one for the equation of state, formulated here for a gas formed by four elements: H, He, a mean element $Z_1$ representative of C, N, O and another mean element $Z_2$ representative of Al, Mg, Si and Ca. (See Cardona et al. 2002.) Here the equation of state yields only a macroscopic description of the gas through the average molecular weight. At each depth point the two blocks are coupled via a simple iterative loop, whose convergence is extraordinarily fast.

The output of the structural macroblock consists of the input temperature $T_i(r)$, the pressure $P(r)$ and the density $\rho(r)$ at each depth point.

2.2. The link between the two macroblocks

The coupling between the structural and the energetic macroblocks is given by the equation of state. Here the microscopical description of the state of the gas yields the degrees of ionization, the atomic populations and the electron density, which enables us to compute the absorption and diffusion coefficients, as well as the thermodynamical coefficients.

2.3. The energetic macroblock

We have now at our disposal all the elements that, together with the temperature $T_i(r)$, constitute the input of the energetic macroblock. The temperature $T_i(r)$, i.e. the primary input of the whole iterative procedure, will be updated inside the energetic macroblocks through a series of internal iterations, during which all the other variables will be kept constant. The correction is twofold: both the radiative and the convective flux are employed separately to yield the new temperature $T(r)$.

The absorption coefficient $a_\nu$ and the diffusion coefficient $\sigma_\nu$, that are invariant input of the macroblock, together with the emission coefficient $\eta_\nu(T) = a_\mu B_\nu(T)$,
that is up-dated at each step of the internal loop, allow us to compute the radiative flux $H_R$.

The thermodynamical coefficients, that are the other invariant input of the macroblock, together with the up-dated temperature $T(r)$, shall yield the convective flux $H_C$, computed by means of a standard mixing-length formula.

The sum $H_R + H_C$ should be equal to the total flux $H$, which is a data of the problem. In general that shall not occur at the first step of iterations. (Otherwise, the solution would have been already achieved.) Thus we shall renormalize the two fluxes:

$$H_R^* = \frac{H_R}{H_R + H_C} H,$$

$$H_C^* = \frac{H_C}{H_R + H_C} H.$$

We will use the values of $H_R^*$ for the radiative temperature correction (cf. Simonneau and Crivellari, 1988 and Simonneau and Crivellari, 1994). By using the values of $H_C^*$ we will perform the convective temperature correction (cf. Crivellari and Simonneau, 1991).

**Fig. 1.** Flowchart of our sequential iterative procedure.
The double temperature correction is iterated until the energy conservation constraint is fulfilled. Then the whole cycle is restarted with the new input temperature $T_i = T_n$.

It is important to stress that the radiative correction of the temperature is performed by solving the radiative equilibrium constraint simultaneously with a new solution of the radiative transfer equation, by employing the method of the iteration factor (Simonneau and Crivellari 1988; Crivellari and Simonneau 1991). Otherwise the sequential solution of the radiative transfer and the energy equilibrium blocks would be equivalent to an ordinary $\Lambda$-iteration, whose severe drawbacks in highly opaque media are well known. (For details, see Crivellari 2002, and also Simonneau and Crivellari 1999.)

3. Preliminary results

For the moment the product of our "laboratory" consits of RE and LTE atmosphere models and the corresponding emergent spectra (computed only at the frequencies that are necessary for the computation of the model).

The quality of the results is proved by the values of the total flux $H$ computed after the convergence of the solution, independently of the method of correction of the temperature. For a grid of models with $1000 < T_{\text{eff}} < 60000 \text{ K}$ and $1 \leq \log g < 5$, at each depth point of the model the conservation of the total flux is achieved with a precision better than 0.2%.

By comparison with the other models nowadays available, to say nothing of the easy direct control on all the components of the algorithmic structure that allows us to experiment different physical instances, it must be remarked that the models of our grid extend from the sub-photospheric regions up to the outermost layers of very shallow optical depth ($\tau_{\text{Rosseland}} \lesssim 10^{-15}$). Such a wide range of layers cannot be covered simultaneously by ordinary models.

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References