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ORIGINAL ARTICLE

CLÉS, Code Liégeois d'Évolution Stellaire

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Abstract CLÉS is an evolution code recently developed to produce stellar models meeting the specific requirements of studies in asteroseismology. It offers the users a lot of choices in the input physics they want in their models and its versatility allows them to tailor the code to their needs and implement easily new features. We describe the features implemented in the current version of the code and the techniques used to solve the equations of stellar structure and evolution. A brief account is given of the use of the program and of a solar calibration realized with it.

Keywords Stars · Stellar structure · Stellar evolution

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1 Introduction

Since the early 70s, the asteroseismology group at the Institute of Astrophysics and Geophysics of Liège has been using an evolution code derived from the Henyey code. This code has been continuously updated. Nevertheless, with the progress of asteroseismology, it became clear that the frequencies and the stability of the oscillation modes were extremely sensitive to details of the model, which were unimportant for the computation of stellar evolution. A few years ago, it was thus decided to write a new code, meeting the specific requirements of our studies in asteroseismology. This code has been named *Clés*, the acronym of *Code Liégeois d'Évolution Stellaire*. It is still in an active phase of development. A number of persons have contributed and contribute to its development. The main objective of this effort is to have a versatile stellar evolution code producing models precise enough to be useful for studies in asteroseismology. We try to maintain a clear structure so that every user will be able to tailor the code to his own needs.

Clés has been developed on a GNU/Linux system (more precisely a Slackware one). No effort has been made to port the software to another platform. It is written in FORTRAN 77. A few relatively standard extensions of the language provided by the GNU Fortran compiler g77 have been used. A few scripts use the Bash shell and the script building the Makefile is a Tcl script.

The present version of the code is numbered 18. The code is not unique. As it is easy to customize, several versions of the code have been developed from the standard version, implementing different features needed by the works already realized or in progress. The most interesting of these will be included in the next standard version of the code so as to preserve its uniqueness. The features described below do not necessary belong to the standard version. After a brief reminder of the equations we have to solve, we describe the physical assumptions. Two sections are then devoted to technical aspects and we end with considerations on the use of Clés, a solar calibration and a brief discussion.

Due to limitations in the physics already implemented, the present version of Clés is not intended for the helium burning phases of the evolution.

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2 Structure and evolution equations

2.1 Structure

The quasi-equilibrium structure of a star is governed by the following equations (we use well-known notations):

$$\frac{\partial P}{\partial r} = -\frac{Gm\rho}{r^2}, \tag{1}$$

$$\frac{\partial m}{\partial r} = 4\pi r^2 \rho, \tag{2}$$

$$\frac{\partial L}{\partial r} = 4\pi r^2 \rho(\varepsilon + \varepsilon_g), \tag{3}$$

$$\frac{\partial T}{\partial r} = -\frac{Gm\rho T}{r^2 P}\nabla. \tag{4}$$

In (3), the luminosity L does not include the neutrino luminosity and the term ε denotes the rate of production of nuclear energy from which we have already excluded the neutrinos losses. In the same equation, the term ε_g deserves a comment. It hides a time derivative and governs the evolution rate when no significant nuclear energy sources are available, for instance in the beginning of the pre-main sequence phase. It reads

$$\varepsilon_g = -\frac{dU}{dt} + \frac{P}{\rho^2}\frac{d\rho}{dt} = -T\frac{dS}{dt} - \sum_i \mu_i \frac{dn_i}{dt}, \tag{5}$$

where μ_i is the chemical potential of element i and n_i the number of moles per gram. In this expression, some people keep only the term $-TdS/dt$ (Kippenhahn and Weigert 1990), but this neglects the effects of changes in chemical composition. An enlightening discussion of the correct form of this term is given by Strittmatter et al. (1970).

In (4), ∇ stands for $d\ln P/d\ln T$ and is computed differently according to whether the considered point belongs to a radiative or convective zone. In a radiative zone, the diffusion approximation allows us to write the temperature gradient as

$$\nabla = \nabla_{\rm rad} = \frac{3\kappa L P}{16\pi acGmT^4}. \tag{6}$$

The expression of ∇ in a convective zone is discussed in the section devoted to convection.

Boundary conditions The differential equations of structure must be supplemented with boundary conditions. The conditions at the center are obvious, m and L must vanish as r^3. In the external layers of the star, the diffusion approximation progressively breaks down as the optical depth approaches unity. Rather than integrating the full radiative problem, it is usual to join smoothly the interior solution to a precomputed atmosphere model, which imposes, in this way, external boundary conditions on the interior model.

2.2 Chemical evolution

The equations governing the rate of change of the abundances of the elements may be written in the form

$$\frac{dX_i}{dt} = \sum_j R_{ij} - \frac{1}{\rho r^2}\frac{\partial}{\partial r}(r^2 \rho X_i w_i). \tag{7}$$

R_{ij} expresses the contribution of the j-th nuclear reaction to the variation of the species i. It depends on the abundances of several species in a non linear way and needs no further explanation. w_i is the diffusion velocity of element i. The computation of this term is described in Sect. 3.6.

In convective and overshooting zones, the different species are rapidly mixed. In a few evolution codes this rapid mixing is described as a diffusive process with appropriate coefficients. In Clés, convective mixing is an instantaneous process and the chemical homogeneity of convective zones is imposed. In a given convective zone, the abundances X_i do not depend on r and (7) is replaced by its integrated form over the entire convective zone:

$$m_c \frac{dX_i}{dt} = \int_{m_1}^{m_2} \sum_j R_{ij}\, dm - (4\pi r^2 \rho X_i w_i)_2 + (4\pi r^2 \rho X_i w_i)_1, \tag{8}$$

where m_c is the mass of the convective zone and indexes 1 and 2 refer to the bottom and the top of the convective zone respectively.

Initial conditions The first model of a sequence is always on the Hayashi track. It is chemically homogeneous and its central temperature is between 4×10^5 and 5×10^5 K. The initial chemical composition is defined by X and Z, the mass fractions of hydrogen and metals. The metal mixture and the isotopic abundances can be changed by the user. It is however his responsibility to select appropriate opacity tables. The standard version of Clés comes with two metal mixtures, GN93 (Grevesse and Noels 1993) and AGS05 (Asplund et al. 2005) and the Anders and Grevesse (1989) isotopic abundances. It must be stressed that for Li, Be and B, contrary to other elements, we do not use solar photospheric abundances. As these elements may have undergone nuclear processing at the basis of the solar convective zone, we have adopted their meteoritic abundances.

3 Input physics

3.1 Equation of state

We do not compute the equation of state (EOS) in the evolution code. A few EOS are provided in the form of precomputed tables which are interpolated. We are particularly

careful with respect to the consistency between the different thermodynamic quantities provided by the equation of state. The independent variables are $\log\rho$, $\log T$, X and Z (log stands for the decimal logarithm). At each grid point, we store only $\log P$, $\log C_v$, $P_\rho = (\partial \log P/\partial \log \rho)_T$ and $P_T = (\partial \log P/\partial \log T)_\rho$ for the gas. In the EOS routine, these quantities are interpolated, the easily computed contribution of the radiation is taken into account and all other thermodynamic quantities are deduced from well-known identities. The contributions of the radiation are included as follows.

$$P = P_{\rm gas} + P_{\rm rad} \quad \text{with } P_{\rm rad} = \frac{1}{3}aT^4, \tag{9}$$

$$C_v = C_{v,\rm gas} + \frac{4aT^3}{\rho}, \tag{10}$$

$$P_\rho = \beta P_{\rho,\rm gas} \quad \text{with } \beta = P_{\rm gas}/P, \tag{11}$$

$$P_T = \beta P_{T,\rm gas} + 4(1-\beta). \tag{12}$$

Adiabatic exponents and C_p are then computed,

$$\Gamma_3 - 1 = \frac{P_T P}{C_v \rho T}, \tag{13}$$

$$\Gamma_1 = P_\rho + (\Gamma_3 - 1) P_T, \tag{14}$$

$$C_p = \Gamma_1 C_v / P_\rho. \tag{15}$$

Three EOS tables have been used with Clés, implementing CEFF (Christensen-Dalsgaard and Däppen 1992), OPAL 2001 and OPAL 2005 (Rogers and Nayfonov 2002). We have computed the CEFF table with a routine kindly provided by J. Christensen-Dalsgaard. A metal mixture defined by the abundances of ten metals can be input to the routine. As the EOS is not very sensitive to the metal mixture, we have computed only one table with a mixture as close as possible to the GN93 mixture. The OPAL 2001 and 2005 EOS are available in tabular form for a fixed metal mixture of four elements (C, N, O and Ne). As the C_v from OPAL 2001 tables are known to be inaccurate (Boothroyd and Sackmann 2003), C_v has been computed from the other tabulated quantities.

For the necessity of diffusion a routine computes the stage of ionization of all the elements involved in the diffusion process (Saha's equation).

3.2 Opacity

The standard version of Clés uses OPAL opacities (Iglesias and Rogers 1996), completed with the opacities of Alexander and Ferguson (1994) at low temperature. Both tables have been smoothly merged into a single table. In the temperature domain $\log T \in [3.9, 4.15]$ where the opacity is defined in both tables, we use an opacity κ defined as the average

$$\log\kappa = (1-\theta)\log\kappa_{\rm AF} + \theta \log\kappa_{\rm OPAL}. \tag{16}$$

In this expression, θ is the unique third degree polynomial in $\log T$, with vanishing derivatives at both ends of the interval and taking zero and unity values at the lower and higher ends respectively.

A few opacity tables have been built for different metal mixtures. Appropriate tools allow the user to build new tables in the format required by Clés from tables generated at the OPAL site and the tables of Alexander and Ferguson. For particular studies, tables using the new Ferguson et al. (2005) opacities and OP opacities (Badnell et al. 2005) have also been built (Miglio et al. 2007b).

For the computation of models with local variations of the metal mixture, several tables with different metal mixtures are loaded and interpolated (Miglio et al. 2007a).

Up to now the effects of conduction on opacities have been neglected.

3.3 Nuclear reactions

The following reactions are included in our nuclear reaction network.

p-p chains:

$$2\ {}^1\mathrm{H} \rightarrow {}^2\mathrm{H} + e^+ + \nu, \tag{17}$$

$${}^2\mathrm{H} + {}^1\mathrm{H} \rightarrow {}^3\mathrm{He} + \gamma, \tag{18}$$

$$2\ {}^3\mathrm{He} \rightarrow {}^4\mathrm{He} + 2\ {}^1\mathrm{H}, \tag{19}$$

$${}^3\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^7\mathrm{Be} + \gamma, \tag{20}$$

$${}^7\mathrm{Be} + e^- \rightarrow {}^7\mathrm{Li} + \nu, \tag{21}$$

$${}^7\mathrm{Li} + {}^1\mathrm{H} \rightarrow 2\ {}^4\mathrm{He}, \tag{22}$$

$${}^7\mathrm{Be} + {}^1\mathrm{H} \rightarrow 2\ {}^4\mathrm{He} + e^+ + \nu + \gamma. \tag{23}$$

CNO cycles:

$${}^{12}\mathrm{C} + {}^1\mathrm{H} \rightarrow {}^{13}\mathrm{C} + e^+ + \nu + \gamma, \tag{24}$$

$${}^{13}\mathrm{C} + {}^1\mathrm{H} \rightarrow {}^{14}\mathrm{N} + \gamma, \tag{25}$$

$${}^{14}\mathrm{N} + {}^1\mathrm{H} \rightarrow {}^{15}\mathrm{N} + e^+ + \nu + \gamma, \tag{26}$$

$${}^{15}\mathrm{N} + {}^1\mathrm{H} \rightarrow {}^{12}\mathrm{C} + {}^4\mathrm{He}, \tag{27}$$

$${}^{15}\mathrm{N} + {}^1\mathrm{H} \rightarrow {}^{16}\mathrm{O} + \gamma, \tag{28}$$

$${}^{16}\mathrm{O} + {}^1\mathrm{H} \rightarrow {}^{17}\mathrm{O} + e^+ + \nu + \gamma, \tag{29}$$

$${}^{17}\mathrm{O} + {}^1\mathrm{H} \rightarrow {}^{14}\mathrm{N} + {}^4\mathrm{He}, \tag{30}$$

$${}^{18}\mathrm{O} + {}^1\mathrm{H} \rightarrow {}^{15}\mathrm{N} + {}^4\mathrm{He}. \tag{31}$$

He combustion:

$$3\ {}^4\mathrm{He} \rightarrow {}^{12}\mathrm{C} + \gamma, \tag{32}$$

$${}^{12}\mathrm{C} + {}^4\mathrm{He} \rightarrow {}^{16}\mathrm{O} + \gamma, \tag{33}$$

$${}^{14}\mathrm{N} + {}^4\mathrm{He} \rightarrow {}^{18}\mathrm{O} + e^+ + \nu + \gamma, \tag{34}$$

$${}^{16}\mathrm{O} + {}^4\mathrm{He} \rightarrow {}^{20}\mathrm{Ne} + \gamma. \tag{35}$$

We follow thoroughly the combustion of ^{2}H and ^{7}Li. Only unstable species (^{7}Be, ^{13}N, ^{15}O, ^{17}F and ^{18}F) are supposed to be at equilibrium. Though the main reactions of the helium burning phase have already been implemented, we have yet to improve our code (semi-convection, equation of state, opacity) to be able to accurately follow this phase of the evolution.

The reaction rates are computed using the analytical expressions given by Caughlan and Fowler (1988). For the reaction ^{14}N(p,γ)^{15}O, we use the cross-section given by Formicola et al. (2004). A variant of the program using the NACRE reaction rates in their approximate analytical form (Angulo et al. 1999) has been written to facilitate the comparisons with CESAM (Montalbán and Lebreton 2005; Montalbán 2005; Montalbán et al. 2005).

The screening factors are computed according to Salpeter (1954).

3.4 Atmosphere

At the last point of a stellar model Clés realizes a smooth junction with a pre-computed model atmosphere. To that end, tables giving the outer boundary conditions in terms of g, T_{eff}, X and Z have been computed from Kurucz atmospheres (Kurucz 1998) at different optical depths (photosphere and $\tau = 1$, 10 and 100). We have also prepared tables of boundary conditions from radiative gray Eddington atmospheres.

3.5 Convection

A region of a star is dynamically stable against convective movements, if Ledoux's criterion is satisfied:

$$\frac{d\ln\rho}{dr} - \frac{1}{\Gamma_1}\frac{d\ln P}{dr} < 0. \tag{36}$$

In a chemically homogeneous zone, it is equivalent to the criterion of Schwarzschild:

$$\nabla_{\mathrm{rad}} < \nabla_{\mathrm{ad}}, \tag{37}$$

where $\nabla_{\mathrm{ad}} = (\Gamma_3 - 1)/\Gamma_1$ is the adiabatic gradient. In presence of a chemical inhomogeneity, both criteria cease to be equivalent. In term of ∇, Ledoux criterion reads

$$\nabla < \nabla_{Ldx}, \tag{38}$$

where ∇_{Ldx} derives from the rewriting of equation (36). It is sufficient for our purpose to give its expression for a completely ionized perfect gas

$$\nabla_{Ldx} = \nabla_{\mathrm{ad}} + \nabla_{\mu}, \tag{39}$$

where $\nabla_{\mu} = d\ln\mu/d\ln P$ is the gradient of the mean atomic weight. For a non homogeneous region to be in radiative stability, it is not enough to satisfy Ledoux's criterion. In that case, Schwarzschild's criterion is a necessary condition for vibrational stability. In a star, due to nuclear processing, the mean atomic weight generally decreases from the centre to the surface and the term ∇_{μ} is positive. We have then

$$\nabla_{\mathrm{ad}} < \nabla_{Ldx}, \tag{40}$$

and when Schwarzschild's criterion is satisfied, Ledoux's one is satisfied too. However, when diffusion is taken into account, gradients may develop in small regions of the star, where this inequality is reversed and Ledoux' criterion must be explicitly taken into account.

We have implemented the usual mixing-length theory of Böhm-Vitense (1958), also exposed in the textbooks of Cox and Giuli (1968) and Kippenhahn and Weigert (1990). It is a local theory, in which the temperature gradient is obtained very simply by solving the cubic equation

$$\frac{9}{4}\Gamma^3 + \Gamma^2 + \Gamma = A(\nabla_{\mathrm{rad}} - \nabla_{\mathrm{ad}}), \tag{41}$$

where A is expressed in terms of the mixing-length ℓ, generally defined as a multiple of the scale-height, $\ell = \alpha H_P$, with coefficient α chosen by the user:

$$A = \frac{P_T\rho}{2P_\rho P}\left[\frac{\kappa C_p \rho^2 g \ell^2}{12acT^3}\right]^2. \tag{42}$$

The real temperature gradient is then expressed as

$$\nabla = \frac{\frac{9}{4}\Gamma^2\nabla_{\mathrm{ad}} + (\Gamma+1)\nabla_{\mathrm{rad}}}{\frac{9}{4}\Gamma^2 + \Gamma + 1}. \tag{43}$$

The variant due to Henyey et al. (1965) has also been used for the description of convection at low optical depth.

The Full Spectrum Turbulence (FST) theory of convection (Canuto and Mazzitelli 1991, 1992), has also been implemented (Miglio and Montalbán 2005).

No effort has been made to put a grid point at the boundary of a convective zone. Though the mixing of the material inside convective zones takes into account the precise location of their boundaries, this results in a small diffusion of numerical origin at the boundaries.

Overshooting Overshooting (or undershooting) displaces the boundary of a mixed region from r_c to r_{ov} given by

$$r_{ov} = r_c \pm \alpha_{ov} \min(H_P, h), \tag{44}$$

where h is the thickness of the convective zone and the overshooting coefficient α_{ov} is chosen by the user.

In the overshooting region, the temperature gradient can be chosen adiabatic (only for the core), radiative or computed according to the prescription of the mixing length theory (Godart 2007).

Semi-convection No semi-convection treatment has been implemented. For low-mass main-sequence stars, this results in an uncertainty on the position of the boundaries of the convective regions, at the limit of the core when it is increasing and also at the bottom of the convective envelope when diffusion is included (Miglio et al. 2005; Montalbán et al. 2007).

3.6 Diffusion

We follow the theory of stellar diffusion developed by Thoul et al. (1994). From their fundamental equations (12), (13), (18) and (19), we eliminate the electron density and express the diffusion velocity w_i in terms of the gradients of abundances of all ions, of pressure and temperature:

$$w_i = \sum_j a_{ij} \frac{dX_j}{dr} + a_P \frac{d\ln P}{dr} + a_T \frac{d\ln T}{dr}. \tag{45}$$

Though it is possible to eliminate one of the ion abundances, it seems that keeping all the abundances ensures a better stability to the solving process.

In the standard version of the code, three groups of elements are distinguished for the treatment of diffusion, hydrogen, helium and the metals. But in the most advanced version of the code, the diffusion of a dozen species is considered: the species involved in the nuclear reaction network (except Li, Be and B), Fe and a fictitious species gathering all the other ones. The mean degree of ionization of each species is computed and the mean charges of the ions are used in the computation of the diffusion coefficients.

Parametric turbulent diffusion has also been implemented (Miglio et al. 2007c) and in one version of the code, radiative forces from the OP project (Seaton 2005) are available (Bourge and Alecian 2006; Bourge et al. 2006, 2007).

3.7 Mass loss

The inclusion of a diffusion process without mass loss leads to overabundances of hydrogen in the external layers. For solar models or stellar models with convective envelopes, this effect is hidden by the mixture due to convection. But for more massive stars, specially when radiative forces are taken into account, it turns out that a slight mass loss, compatible with admitted values, (of the order of 10^{-9} $M_\odot$/yr for a 10 $M_\odot$ star) is necessary to prevent the building of unrealistic abundances in the external layers of the star and has been implemented (Bourge et al. 2007). Work is in progress to cope with higher mass losses encountered in more massive stars.

4 Discretization

The physical quantities describing the star are recorded at a number of discrete points. Though their numbers can vary during the course of evolution (by addition or deletion), these points are linked to a given material element of the star, in other words, as long as point P_k is not deleted, the value of m_k is preserved. In fact, the fundamental quantities used to characterize our Lagrangian grid are not the m_k but the masses of the shells between the grid points $m_{k+1} - m_k$, for the sake of precision in the external layers.

4.1 Structure

At each epoch t, a model is computed by solving the following difference equations:

$$P_{k+1} - P_k = \frac{1}{2}\left[\left(\frac{dP}{dr}\right)_k + \left(\frac{dP}{dr}\right)_{k+1}\right](r_{k+1} - r_k), \tag{46}$$

$$m_{k+1} - m_k = \frac{1}{2}(\rho_k + \rho_{k+1})(V_{k+1} - V_k), \tag{47}$$

$$L_{k+1} - L_k = \frac{1}{2}(\varepsilon_k + \varepsilon_{g,k} + \varepsilon_{k+1} + \varepsilon_{g,k+1}) \times (m_{k+1} - m_k), \tag{48}$$

$$T_{k+1} - T_k = \frac{1}{2}\left[\left(\frac{dT}{dr}\right)_k + \left(\frac{dT}{dr}\right)_{k+1}\right](r_{k+1} - r_k), \tag{49}$$

with $V = 4\pi r^3/3$. In the energy equation (48), the ε_g terms involve differences between quantities at epoch t and $t - \delta t$. Omitting index k,

$$\varepsilon_g = \left\{-C_v(T - T^0) + \frac{(\Gamma_3 - 1)C_v T}{\rho}(\rho - \rho^0) - \frac{3}{2}\mathcal{R}T[2(X - X^0) + 0.75(Y - Y^0) + 0.5(Z - Z^0)]\right\} \Big/ \delta t, \tag{50}$$

where upper index 0 refers to the model at epoch $t - \delta t$.

4.2 Chemical evolution

We update the chemical composition in a two-step process. The change of composition due to diffusion is first computed. In a second step, the change of composition due to nuclear burning and mixing are computed simultaneously. This two-step process reflects the history of the development of the code (diffusion was not included in the first versions) and will be corrected in future versions. Fortunately, the diffusion process turns out to be fast only in the external layers of the star where there is no nuclear burning. The code is not able to follow the evolution of Li, Be and B.

Diffusion In certain circumstances, the diffusion is fast enough in the external layers, so that the time scale of the diffusion is smaller than any reasonable timestep (stiff differential equations). In such cases, numerical stability of the discrete scheme requires that the second members of the evolution equations (7) be calculated using the updated values.

With index i referring to the chemical species, index k to the grid point and upper index 0 to the previous epoch $t-\delta t$, our discrete equations may be written (omitting unimportant details linked to the non equidistance of the mesh points)

$$\frac{X_{ik}-X_{ik}^0}{\delta t} = -\{(4\pi r^2 \rho X_i w_i)_{k+1/2} - (4\pi r^2 \rho X_i w_i)_{k-1/2}\} /(m_{k+1/2}-m_{k-1/2}), \tag{51}$$

$$w_{i,k+1/2} = \Big\{\sum_j a_{ij,k+1/2}(X_{j,k+1}-X_{jk}) + a_{P,k+1/2}(\ln P_{k+1}-\ln P_k) + a_{T,k+1/2}(\ln T_{k+1}-\ln T_k)\Big\} \Big/ (r_{k+1}-r_k), \tag{52}$$

where the fractional values of the spatial index have obvious meaning:

$$r_{k+1/2} = (r_k + r_{k+1})/2, \quad \ldots \tag{53}$$

Nuclear reactions The life-time of the different nuclear species are of very different orders of magnitude, with some of them very much shorter than the timestep. We apply the same technique as described in the previous paragraph to this stiff differential system. As the life-time of hydrogen is of roughly the same order as the duration of the main sequence, it is possible (and that gives better approximation) to use an average abundance of hydrogen $\bar{X} = (X + X^0)/2$ in the second member. This possibility has not been used in Clés:

$$\frac{X_{ik}-X_{ik}^0}{\delta t} = \sum_j R_{ijk}, \tag{54}$$

where the indices have the same meaning as above, except that index 0 refers now to the abundances obtained after the diffusion step.

In a convective zone, the X_{ik} are equal for all points k in the zone and (54) must be replaced by the discretized form of (8). However a simple and direct discretization would produce unphysical discontinuities when a convective zone recedes by more than one spatial interval in one timestep. A dedicated algorithm has been implemented to produce a continuous chemical profile in this case.

5 Implementation

5.1 The general structure

Stancliffe (2006) distinguishes three different strategies for a stellar evolution code to advance by one timestep. Our code falls in his *partially simultaneous* category. A timestep begins with an updating of the chemical composition followed by solving the structure equations. These two processes are then repeated until convergence.

Updating the chemical composition The discretized equations of evolution are nonlinear. They are solved with the Newton–Raphson algorithm. We use the composition of the previous model as a first guess.

Solving the structure equations The structure equations are solved by the Newton–Raphson algorithm. When it gives signs of difficult convergence, we apply only a fraction of the correction suggested by the algorithm and when this recipe fails, we adopt a smaller timestep. In the present state of the code, we use the last computed model as a first guess to start the iteration. We could probably improve the rate of convergence by using an extrapolation of the last two computed models as first guess.

5.2 Interpolation in tables

To guarantee the continuity of interpolated functions as well as their first derivatives, we use cubic splines. In 1-D, continuity of the second derivative can be achieved with cubic splines. However, this results in non-local and sometimes unphysical behavior of the interpolating function. We prefer to be able to impose the values of the first derivative at the grid points, values that we compute locally (involving only three points), and therefore we sacrifice the continuity of the second derivative. This interpolation strategy can be extended to more than one dimension in several ways. When interpolating physical data, affected by their inherent uncertainties, it seems that the choice between the different variants is unimportant. The interpolation is faster if the derivatives are stored with the values, but the tables occupy more space in memory. Both strategies have been used in Clés, we tend now to favor the gain in computing time.

5.3 Choice of the grid

The grid of points of the model is adapted during the evolution in such a way as to limit the variations of different physical quantities from one point to its neighbors. The controlled variables are r, m, P and T. The grid of one model is obtained from the grid of the previous one, with addition or deletion of points so that the following rules are satisfied: $\Delta r \leq 5 \times 10^{-3} R$, $\Delta m \leq 5 \times 10^{-3} M$, $\Delta P \leq 5 \times 10^{-2} P$ and $\Delta T \leq 10^{-2}$. A simple command allows the user to impose stricter or looser rules for the grid choice.

With the default rules, a 2 $M_\odot$ model typically starts on the Hayashi track with 700 points, reaches the zero-age main sequence with 1150 points and keeps about the same number of points along the main sequence with local additions and deletions.

5.4 Choice of the timestep

The timestep is chosen small enough to ensure that selected physical quantities do not vary too much from one model to the next one. The controlled variables are the local values of T, P and L and the central hydrogen abundance X_c. The allowed maximum variations depend on the evolution stage and are read from a table. This strategy gives the flexibility to adopt less severe criteria for the pre-main sequence computation for instance. However, when the Newton–Raphson algorithm fails to converge, the timestep is halved. The user has the possibility to influence, in a certain measure, the choice of the timestep.

With no intervention of the user, a 2 $M_\odot$ model evolution needs 125 steps for the pre-main sequence, 75 steps for the main sequence and 20 steps more for the second gravitational contraction.

However, for evolution sequences computed with diffusion, the timestep is effectively controlled by the necessity of convergence of the diffusion algorithm.

5.5 First model

When the luminosity of the star is mainly powered by the nuclear reactions, it is enough to give the chemical composition as a function of the mass, $X_i(m)$ to characterize a model. The good model will not be far from the model obtained by solving the structure equation with $\varepsilon_g = 0$. This is not true for our first model on the Hayashi sequence. To characterize it completely, we have to impose, for instance, its luminosity and assume that it is contracting in a homologous way.

6 The use of Clés

There are different levels of sophistication in the use of Clés.

When it starts, Clés reads a command file, i.e. a succession of commands composed of a keyword followed by parameters, instructing the program of the task it has to perform: mass of the star, chemical composition, EOS table, opacity table, convection parameter,... Clés supplies default values for the parameters not specified by the user. The basic user must just know how to write a command file to express his requirements. This is well explained in a *User's Guide* of ten or so pages.

The next step in the use of Clés consists in providing the program with new tables, such as opacities for a new metal mixture. Tools are available to help the user in this task.

The more informed user may need to test conditions during the evolution and interact with the program. A subroutine called `clesuser`, which does nothing in the standard version of the program, can be customized to meet the need of the user. It is called by the program before each timestep and gives the user the opportunity to read or modify the last computed model or the parameters used for the computation.

At last, a few users have implemented in their copy of the code the features needed for their particular research. This is facilitated by the modular structure of the code.

7 Calibration of solar models

The solar models are calibrated by adjusting the mixing-length parameter α, the initial mass fraction X_0 of hydrogen and the initial mass fraction Z_0 of heavy elements in order to reproduce, at the solar age (4.57×10^9 yr, Bahcall et al. 1995): the observed luminosity (3.842×10^{33} erg s^{-1}, Bahcall et al. 2001, radius (6.9599×10^{10} cm, Allen 1973) and ratio of heavy elements to hydrogen in the photosphere ($Z/X = 0.0245$, Grevesse and Noels 1993). In the solar calibration we adopt a spatial and temporal discretization finer than the standard one (see Sect. 5): the number of meshpoints in a solar model is typically ∼2500 and ∼350 timesteps are needed to reach the solar age (including the pre-main sequence phase).

As the values of the calibrated parameters depend on the choice of the physical inputs, as an example we here present two solar models computed with different opacity tables: OPAL (Iglesias and Rogers 1996) and the recent OP opacities (Seaton 2005) both complemented at low temperature with Ferguson et al. (2005) opacities. The remaining common physical inputs are: the mixing-length theory for convection, GN93 (Grevesse and Noels 1993) metal mixture, NACRE+Formicola et al. (2004) nuclear reaction rates and the OPAL 2001 equation of state (Rogers and Nayfonov 2002). The outer boundary condition is given by a radiative gray Eddington atmosphere computed using Ferguson et al. (2005) opacities. The models include microscopic diffusion of H, He and Z as in the standard version of the code (see Sect. 3.6).

Table 1 Parameters of calibrated solar models. The normalized radius at the base of the convective envelope r_{cz} and the surface helium abundance (Y_S) are also reported. The values of these parameters obtained by helioseismology are respectively 0.713 ± 0.001 (Basu and Antia 1997) and 0.245 ± 0.005 (Boothroyd and Sackmann 2003)

Model	α	X_0	Z_0	r_{cz}	Y_s
OPAL	1.805	0.7043	0.0201	0.7156	0.2450
OP	1.818	0.7056	0.0201	0.7133	0.2442

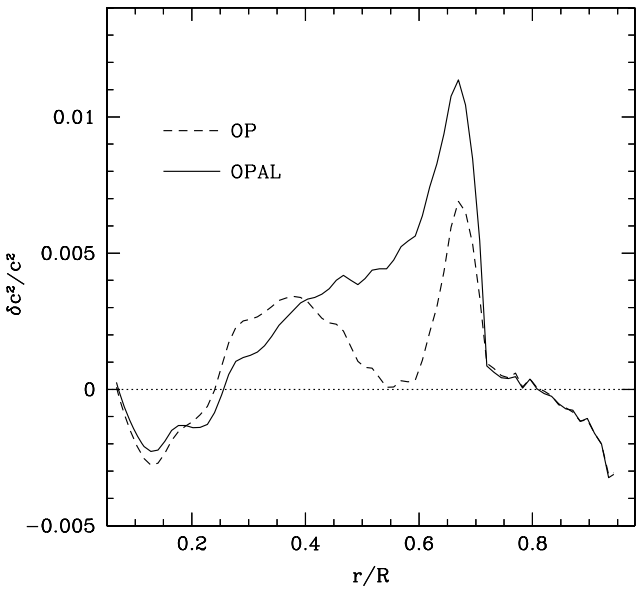

Fig. 1 Relative differences in the squared sound speed between the calibrated models and the Sun (Basu et al. 2000)

The parameters resulting from the calibration are reported in Table 1, along with the normalized radius of the convective envelope and the helium abundance in the envelope. The relative differences in the squared sound speed inferred from helioseismic inversion (Basu et al. 2000) is shown in Fig. 1.

8 Discussion

From the standard version 18 of Clés, a few users/developers working in close collaboration in the Asteroseismology Group of Liège have implemented a number of desirable features in the code. At the moment, there is no single copy of the code implementing all the features described above. Our first goal is now to gather the most significant developments already achieved and a few more in a unique version 19. And we hope that this cycle of development will be repeated to create new versions.

This strategy of development was made possible because the developers have been working in close collaboration on the same site. In less favorable circumstances, it would require a good documentation. Unfortunately, this is not the case, except for a user's manual. We are still far from the ideal situation described by Hut (2006) but we will make the writing of a good documentation our second priority.

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