Clés, Code Liégeois d'Évolution Stellaire

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Introduction

Since the early 70s, our research group at the Institute of Astrophysics 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 too sensitive to details of the model, which were unimportant for the computation of stellar evolution. It was thus decided to write a new code, meeting the specific requirements of our studies in asteroseismology. This code has been named *Clés*. It is the acronym of *Code Liégeois d'Évolution Stellaire*. It is still in an active phase of development. The code is intended to be easily customized to the needs of the user and Josefina Montalban has created some variants of it for the needs of the comparison with CESAM. I will briefly describe some features of the current version (version 18) and say a few words about the developments in progress. I will mainly insist on some aspects of the code and differences with CESAM, which may be useful to understand the results of the comparisons of models computed with the two codes, a subject that will be discussed by Josefina Montalban and Yveline Lebreton in this meeting.

Numerics

Clés is a lagrangian code. Finite difference equations of order two are used for the discretization of the spatial equations. The mesh is automatically adapted so as to limit the variations of physical variables from one point to the next one. The default criteria used to choose the mesh size are

$$\Delta r/R \leq 5\times10^{-3}\,,\ \Delta m/M \leq 5\times10^{-3}\,,\ \Delta P/P \leq 5\times10^{-2} \text{ and } \Delta T/T \leq 10^{-2}\,.$$

Unfortunately, no effort has been made to increase the number of points near the boundaries of convective zones. With these criteria, a 2 $M_\odot$ model starts its evolution on the Hayashi track with 700 points and reaches the zero-age main sequence with 1150 points. The same total number of points is approximately kept along the main sequence, with local additions or deletions of points. A simple command allows the user to require a finer or a coarser mesh.

The finite difference scheme written to follow the time evolution of the abundances is of order one to avoid numerical instabilities. The timestep is chosen to limit the variations of the physical variables from one model to the next. For instance, for a 2 $M_\odot$ model in

its PMS or MS phases, the following default limitations are imposed on the variations of the physical variables from one model to the next.

	$\Delta T/T$	$\Delta P/P$	$\Delta T_e/T_e$	$\Delta L/L$	ΔX_c
if $T_c \leq 1.6 \times 10^7$	4.0×10^{-1}	5.0×10^{-1}	4.0×10^{-2}	1.0×10^{-1}	1.0×10^{-2}
if $T_c > 1.6 \times 10^7$	5.0×10^{-2}	7.0×10^{-2}	7.0×10^{-3}	3.0×10^{-2}	1.0×10^{-2}

The evolution sequences are normally started on the Hayashi sequence. With the above criteria, a 2 $M_\odot$ model evolution needs 125 steps for the pre-main sequence, 75 steps for the main sequence and 20 steps for the second gravitational contraction.

The timestep may be increased or decreased according to the needs of the user. It is also automatically reduced when the resolution of the spatial equations becomes too slow.

Equation of state

Two equations of state (EOS) are implemented, CEFF (Christensen-Dalsgaard and Däppen 1992) and OPAL 2001 (Rogers et al. 1996, Rogers 2001). OPAL comes in tabular form, but tables have also been built for the CEFF EOS (to accelerate the computation). We were not satisfied with the OPAL interpolation routines. We use our own interpolation routines which ensure the continuity of the first derivatives at cell boundaries in the four-dimensional space defined by the variables $\log \rho$, $\log T$, X and Z. The detailed metal mixture is supposed to be unimportant for the EOS (and cannot be changed for OPAL).

Opacity

Clés uses the OPAL opacities (Iglesias and Rogers 1996), completed with the opacities of Alexander and Ferguson (1994) ones at low temperature. The tables are merged in a smooth way. In the temperature domain $\log T \in [3.9, 4.15]$ where the opacity is defined in both tables, Clés uses an opacity κ defined as the average

$$\log \kappa = (1 - \theta) \log \kappa_{AF} + \theta \log \kappa_{OPAL} \, ,$$

where θ is the third degree polynomial in $\log T$ illustrated in Fig 1.

Again we use our own interpolation routines in the four variables $\log R$, $\log T$, X and Z, where $R = \rho / T_6^3$. At the present time, the metal mixture is fixed for the computation of the opacity, within a given model. A few tables are available for different metal mixtures and new tables are easily computed.

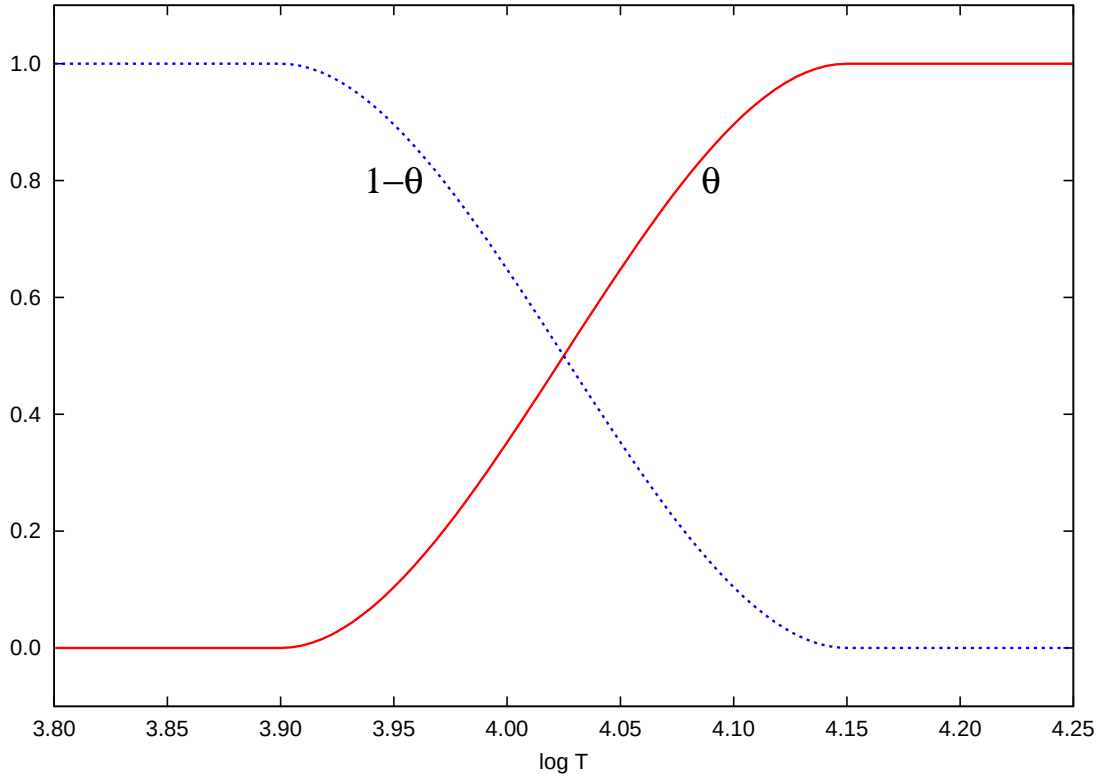

Figure 1: The opacities of Alexander and Ferguson (1994) and OPAL are merged using the function θ.

Nuclear energy generation

The following reactions are taken into account in Clés.

p-p chains:

$$
\begin{gathered}
2\ {}^{1}\mathrm{H} \rightarrow {}^{2}\mathrm{H} + e^{+} + \nu \\
{}^{2}\mathrm{H} + {}^{1}\mathrm{H} \rightarrow {}^{3}\mathrm{He} + \gamma \\
2\ {}^{3}\mathrm{He} \rightarrow {}^{4}\mathrm{He} + 2\ {}^{1}H \\
{}^{3}\mathrm{He} + {}^{4}\mathrm{He} \rightarrow {}^{7}\mathrm{Be} + \gamma \\
{}^{7}\mathrm{Be} + e^{-} \rightarrow {}^{7}\mathrm{Li} + \nu \\
{}^{7}\mathrm{Li} + {}^{1}\mathrm{H} \rightarrow 2\ {}^{4}\mathrm{He} \\
{}^{7}\mathrm{Be} + {}^{1}\mathrm{H} \rightarrow 2\ {}^{4}\mathrm{He} + e^{+} + \nu + \gamma
\end{gathered}
$$

CNO cycles:

$$
\begin{gathered}
{}^{12}\mathrm{C} + {}^{1}\mathrm{H} \rightarrow {}^{13}\mathrm{C} + e^{+} + \nu + \gamma \\
{}^{13}\mathrm{C} + {}^{1}\mathrm{H} \rightarrow {}^{14}\mathrm{N} + \gamma \\
{}^{14}\mathrm{N} + {}^{1}\mathrm{H} \rightarrow {}^{15}\mathrm{N} + e^{+} + \nu + \gamma \\
{}^{15}\mathrm{N} + {}^{1}\mathrm{H} \rightarrow {}^{12}\mathrm{C} + {}^{4}\mathrm{He} \\
{}^{15}\mathrm{N} + {}^{1}\mathrm{H} \rightarrow {}^{16}\mathrm{O} + \gamma \\
{}^{16}\mathrm{O} + {}^{1}\mathrm{H} \rightarrow {}^{17}\mathrm{O} + e^{+} + \nu + \gamma \\
{}^{17}\mathrm{O} + {}^{1}\mathrm{H} \rightarrow {}^{14}\mathrm{N} + {}^{4}\mathrm{He} \\
{}^{18}\mathrm{O} + {}^{1}\mathrm{H} \rightarrow {}^{15}\mathrm{N} + {}^{4}\mathrm{He}
\end{gathered}
$$

He combustion:

$$3\ {}^4\mathrm{He} \rightarrow {}^{12}\mathrm{C} + \gamma$$
$${}^{12}\mathrm{C} + {}^4\mathrm{He} \rightarrow {}^{16}\mathrm{O} + \gamma$$
$${}^{14}\mathrm{N} + {}^4\mathrm{He} \rightarrow {}^{18}\mathrm{O} + e^+ + \nu + \gamma$$
$${}^{16}\mathrm{O} + {}^4\mathrm{He} \rightarrow {}^{20}\mathrm{Ne} + \gamma$$

We follow thoroughly the combustion of ^{2}H and ^{7}Li. Only unstable species (as ^{7}Be, ^{13}N, ^{15}O and ^{17}F) are supposed to be at equilibrium.

We have already implemented the main reactions of the helium burning phase but we have yet to improve our code to be able to accurately follow this phase of the evolution (semi-convection, equation of state, opacity).

The Caughlan and Fowler (1988) reaction rates have been used. For ^{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.

The next version of Clés will use NACRE tables instead of analytical fits.

Gravitational energy generation

There are two different versions of this term in textbooks. In Cox and Giuli (1968) for instance, we find

$$\epsilon_g = -T\frac{dS}{dt} - \sum_i \mu_i \frac{dn_i}{dt}\,,$$

where the μ_i are the chemical potentials and the n_i the number of moles per gram. In Kippenhahn and Weigert (1990) we find

$$\epsilon_g = -T\frac{dS}{dt}\,.$$

The difference between both expressions is not negligible. If we integrate during the whole main sequence, the difference is of the order of the local internal energy. There is a very convincing paper of Strittmatter et al. (1970) in favor of the first expression, which can also be written

$$\epsilon_g = \frac{dU}{dt} - P\frac{d(1/\rho)}{dt}\,.$$

We have adopted this form of ϵ_g in the current version of Clés.

Convection

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).

Henyey et al. (1965) have described a variant which has been totally or partially implemented in some evolution codes, but not in ours. In order to describe possible differences between evolution codes, it is necessary to have a look at some details of the equations.

In a convective zone, it is usual to define four gradients: $\nabla_{rad} > \nabla > \nabla' > \nabla_{ad}$. To determine ∇ in terms of ∇_{rad} and ∇_{ad}, one must solve a cubic equation in Γ, the efficiency of convection (defined as the ratio of the energy effectively transported by convective elements to the energy they loose by radiation). In the Böhm-Vitense theory, this equation reads

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

where the mixing-length parameter enters the definition of coefficient B. Each term of the left-hand side of this equation is linked to a gradient difference,

$$\frac{9}{4}\Gamma^3 = B(\nabla_{rad} - \nabla)\,, \quad \Gamma^2 = B(\nabla - \nabla')\,, \quad \Gamma = B(\nabla' - \nabla_{ad})\,.$$

From these relations the actual gradient in the convective zone can be expressed as

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

The variant of the theory due to Henyey et al. (1965) differs from the standard theory on the following points.

- The turbulent pressure is included in the total pressure and is taken into account in a corrected adiabatic gradient ∇^*_{ad}.
- The departure from the radiative diffusion approximation is taken into account through a corrective factor f. It differs significantly from 1 in the external layers where the optical depth is small.
- The 9/4 factor in the cubic equation is replaced by a factor ϕ which depends on f and on the shape and optical thickness of the convective element.

With these modifications the main equations read

$$\phi\Gamma^3 + \Gamma^2 + \Gamma = B(f\nabla_{rad} - \nabla^*_{ad})\,,$$

$$\nabla = \frac{\phi\Gamma^2\nabla^*_{ad} + (\Gamma+1)f\nabla_{rad}}{\phi\Gamma^2 + \Gamma + 1}\,.$$

According to CESAM 5 user's manual (Morel 2003, description of routines `conv_jmj` and `conv_a0`), the Henyey et al. variant is partially implemented in CESAM. The turbulent pressure is taken into account, but the cubic equation is written without the parameter f. The user's manual gives $\phi = 9/4$ but, in the code, the optical thickness of the convective element is taken into account for the computation of ϕ, with $\phi \to 9/4$ when this optical thickness $\gg 1$.

Another difference between Clés and CESAM in the treatment of convection is the choice of the mixing-length ℓ. It is generally defined as

$$\ell = \alpha H_P\,.$$

In Clés, its value is reduced in thin convective zones in the following way,

$$\ell = \alpha \min(H_P, h)\,,$$

where h is the thickness of the convective zone. In CESAM, the value of ℓ is modified in a more subtle way and vanishes at the boundaries of convective zones.

Presently, the mesh is not adapted to a rigourous treatment of the boundaries of the convective zones. This results in some *numerical diffusion* at the boundaries. This does not seem to be a major problem but we plan to better describe these boundaries with double mesh points in a future version of the code.

Overshooting

In previous versions of Clés, the boundary of the overshooting zone was determined as the point where the pressure is

$$\ln P_{ov} = \ln P_c \pm \alpha_{ov}\,,$$

where P_c is the pressure at the boundary of the convective zone and α_{ov} the overshooting parameter.

In the present version, the extension of the overshooting zone is defined in a more conventional way as

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

where r_c is the radius at the boundary of the convective zone and h its size.

In our models, the gradient in overshooting zones is taken as the radiative gradient ∇_{rad}, whereas in CESAM it is taken as the adiabatic gradient ∇_{ad}.

Diffusion

We follow the theory of stellar diffusion developed by Thoul et al. (1994). A rather crude treatment neglecting the radiative forces is presently implemented. Pierre-Olivier Bourge, one of our PhD student, in collaboration with Georges Alecian, is implementing a treatment taking radiative forces into account in a particular version of the code.

Atmosphere

The models computed by Clés extend up to the photosphere or an optical depth $\tau = 1$, 10 or 100 chosen by the user where they are fitted to a model atmosphere of Kurucz with overshooting (1998). A grey Eddington atmosphere (without convection) can also be fitted at the photospheric level.

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