COMPARISONS FOR ESTA-TASK3: CLES AND CESAM

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Abstract. We present the results of comparing three different implementations of the microscopic diffusion process in the stellar evolution codes CESAM and CLES. For each of these implementations we computed models of 1.0, 1.2 and 1.3 M\textsubscript{\odot}. We analyse the differences in their internal structure at three selected evolutionary stages, as well as the variations of helium abundance and depth of the stellar convective envelope. The origin of these differences and their effects on the seismic properties of the models are also considered.

1 Introduction

As reported in Monteiro \textit{et al.} (2006, and references therein), the stellar models provided by the codes CESAM2k (Morel, 1997) and CLES (Scuflaire \textit{et al.}, 2007a) for a given set of standard input physics, differ by less than 0.5%. At variance with previous comparisons, in this new ESTA-TASK3 we deal with stellar models that include microscopic diffusion. The treatment of the microscopic diffusion process in the evolution codes we test here, is not exactly the same. CLES code computes the diffusion coefficients by solving the Burgers’ equations (Burgers, 1969) with the formalism developed in Thoul \textit{et al.} (1994, thereafter TBL94). CESAM2k provides two approaches to compute diffusion velocities: one (which we will call CESAM2k MP) is based on Michaud & Proffitt (1993) approximation, the other (hereafter CESAM2k B) is based on the Bugers’ formalism, with collision integrals derived from Paquette \textit{et al.} (1986).

We will compare three sets of models Task3.1 (1.0 M\textsubscript{\odot}), Task3.2 (1.2 M\textsubscript{\odot}) and Task3.3 (1.3 M\textsubscript{\odot}), whose input parameters and physics specifications are described in Lebreton (2007). In the next sections we will present the results of comparing the stellar models that were calculated by CLES, CESAM2k MP and CESAM2k B for the three sets of models, and we try to find out the reason of the differences we get.

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DOI: (will be inserted later)
2 Stellar structure and evolution

For each Task3 we select three evolutionary stages: A: a main sequence stage with a central hydrogen content $X_c = 0.35$; B: a stage close to the core hydrogen exhaustion $X_c = 0.01$, and C: a post-main sequence stage in which the mass of the helium core (defined as the central region where the hydrogen mass fraction is $X \leq 0.01$) is $M_{He}^c = 0.05 M_\odot$. CESAM stellar models have a number of mesh points between 2700 and 3100, depending on the evolutionary stage, while CLES models have about 2400 mesh points. Moreover, for all the models considered in these comparisons, the stellar structure ends at $T = T_{eff}$. Concerning the time step, both codes make from 1000 to 1500 (depending on the stellar mass) time steps to reach stage C, and the specifications for the stages A, B and C are achieved with a precision better than $1 \times 10^{-4}$.

Fig. 1 displays, for each microscopic diffusion implementation, the evolutionary tracks for Task3.1, 3.2 and 3.3, and the HR diagram location of the target models.
Fig. 2. Evolution of helium content in the convective envelope ($Y_S$ vs. $X_c$) for 1.0 $M_\odot$ (left panel), 1.2 $M_\odot$ (central panel) and 1.3 $M_\odot$ (right panel).

A, B and C. For each stellar mass, the main sequence computed with CESAM2k B is slightly hotter ($\sim 0.1\%$ for task3.1, to $0.3\%$ for task3.2 and 3.3) than those calculated by CESAM2k MP and CLES. Furthermore, CLES and CESAM2k MP models are quite close ($\Delta R/R < 0.3\%$, and $\Delta L/L < 0.4\%$) with the exception of models in the second overall contraction phase, for which the differences can reach $1\%$ in the stellar radius and $0.5\%$ in luminosity. The fact that CESAM2k B models are hotter than CESAM2k MP and CLES ones could suggest that the outer layer opacity for the former is lower than for the latter because of a different content of hydrogen in their convective envelope. The evolution of the helium abundance in the stellar convective envelope ($Y_S$) is an eloquent indicator of the microscopic diffusion effects. Fig. 2 shows, for each considered stellar mass and diffusion treatment, the variation of $Y_S$ as the central hydrogen content $X_c$ decreases, and reveals that the diffusion efficiency in CLES is always larger than in CESAM: about 8, 10 and 20% larger than in CESAM2k MP for 1.0, 1.2 and 1.3 $M_\odot$ respectively, and 40% larger than in CESAM2k B for all stellar masses under consideration.

The irregular behaviour of $Y_S$ vs. $X_c$ curves for task3.2 and 3.3, is a consequence of a semiconvection phenomenon that appears below the convective envelope and, the longer main sequence for CESAM2k MP models is probably due to semiconvection at the border of the convective core (see next section).

The internal structure at the given stages A, B and C can be studied by means of the sound speed, $c$, and of the adiabatic exponent, $\Gamma_1$, variations. The Lagrangian differences, $d\ln c$ and $d\ln \Gamma_1$, between CESAM2k (both B and MP) and CLES models (calculated at the same mass by using the ADIPLS package tool\cite{adiplstool}) are plotted in Fig. 3 as a function of the normalised radius. Note that the vertical scale in $d\ln c$ and $d\ln \Gamma_1$ plots are respectively five and three times smaller for 1.0 $M_\odot$ than for 1.2 and 1.3 $M_\odot$. The $d\ln c$ values reflect: i) the differences in stellar radius (note that the largest values are reached in Task3.2 B CLES-

\footnote{http://astro.phys.au.dk/~jdc/adipack.n}
Fig. 3. Lagrangian differences of sound speed ($d\ln c$) (upper panels) and adiabatic exponent ($d\ln \Gamma_1$) (lower panels) as a function of the normalised stellar radius for models corresponding to task3.1 (left), task3.2 (centre), task3.3 (right). For each mass, three evolutionary stages are considered: A, with $X_c = 0.35$ (solid lines), B, with $X_c = 0.01$ (dotted lines), and C, with $M_{cHe} = 0.05M_\odot$ (dashed lines).
CESAM2k MP comparison, for which $d\ln R$ is of the order of 0.01; i) the different chemical composition gradients below the convective envelope (features between $r/R = 0.6$ and 0.8), as well as differences in the location of convection region boundaries (at $r/R \sim 0.05$ for the convective core in Task3.2 and 3.3).

The value of $\Gamma_1$ in the external regions is particularly sensitive to the He abundance. Therefore, as one can see in the bottom panels of Fig. 3, the variations $d\ln \Gamma_1$ are smaller for CESAM2k MP–CLES comparisons than for CESAM2k B–CLES ones, and these differences increase with the mass of the model; these results are in good agreement with what we would expect from $Y_S$ curves in Fig. 2.

To clarify how all these differences affect the seismic properties of the models, we compute by means of the adiabatic seismic code LOSC (Scuflaire et al., 2007b) the frequencies of oscillations of all the models at the evolutionary stage A (main sequence models). In Fig. 4 the frequency differences between CLES and CESAM models of 1.2 (left panel) and 1.3 $M_\odot$ (right panel) are shown for $p$-modes with degrees $\ell = 0$, 1, 2, 3. The similar behaviour of curves with different degree indicates that the observed frequency differences reflect mainly the near surface difference of the models. In particular, the oscillatory component in CLES-CESAM2k B frequency differences is the characteristic signature of the different He content in the convective envelope. Note that the vertical scale in both panels is not the same, and that the amplitude of the oscillatory component is related to the difference of surface He content. Comparisons for 1.0 $M_\odot$ models showed frequency differences of about 0.4 $\mu$Hz.

![Fig. 4. Plots of the frequency differences after removing the scaling due to stellar radius, between models computed with CLES and CESAM2k B (dotted lines) and with CLES and CESAM2k MP (solid lines). For each couple CLES-CESAM there are four curves that correspond to different degrees $\ell = 0, 1, 2, 3$. Left panel: 1.2 $M_\odot$ models with $X_c = 0.35$ Right panel: like left panel for 1.3 $M_\odot$ models.](image-url)
3 Boundaries of the convective regions

The evolution of the convective region boundaries in models with metal diffusion is difficult to study. In fact, as it was already noted by Bahcall et al. (2001) in the case of 1.0 M⊙ models, the accumulation of metals below the convective envelope can trigger the onset of semiconvection. As the metal abundance increases below the convection region, the opacity locally increases and the affected layers end up by becoming convectively unstable. The evolution of these unstable layers strongly depends on the numerical treatment of convection borders used in the stellar evolution code. CLES does not treat semiconvection, and the algorithm computing the chemical composition in convective regions includes a kind of “numerical diffusion”. In CLES, the convectively unstable shells may grow and eventually join the convective envelope. As a consequence, the latter becomes suddenly deeper, destroys the Z gradient, recedes, and the process starts again. So, the crinkled profiles of Ys for Task3.2 and 3.3 are a consequence of the sudden variations of the depth of the convective envelope. Since the timescale of diffusion decreases as the mass of the convective envelope decreases, semiconvection appears earlier in 1.3 M⊙ than in 1.2 M⊙ models. Furthermore, in contrast with Bahcall et al. (2001) results, semiconvection does not appear in our evolved 1.0 M⊙ models, probably because of the effect of “numerical diffusion” that reduces the efficiency of metal accumulation. All these effects can be seen in Fig. 5. In Fig. 6 we plot the evolution of the convective envelope for CESAM models. The different treatment of convection borders in both codes leads to different depth of the convective envelope. At Xc = 0.05, CLES models have convective envelopes of about 0.1% deeper than CESAM2k B ones, and of about 2.3%, 0.6% and 0.4% shallower than CESAM2k MP models for 1.0, 1.2 and 1.3 M⊙ respectively.

\[^2\text{We recall that we use the classical Schwarzschild criterion for convective instability.}\]
Fig. 6. Evolution of the radius of the convective envelope for 1.0, 1.2, and 1.3 M⊙ CESAM models. Solid lines correspond to CESAM2k with Burgers equations, and dotted lines to CESAM2k with Michaud & Proffitt (1993).

Fig. 7. Convective core mass evolution for 1.2 M⊙ evolution computed with CLES (left panel) and with CESAM (right panel). The black region in left panel correspond to the convective core, and grey ones are convectively unstable regions outside the convective core.

Semiconvection can also appear at the border of the convective core. As explained in Richard et al. (2001), because of the He abundance gradient generated at the border of the convective core by nuclear burning, the diffusion term due
to the composition gradient counteracts the He settling term and He ends up by going out of the core. Since the outward He flux interacts also with the metals, these may as well diffuse outward the core and prevent the metals settling. The enhancement of metals at the border of the convective core induces an increase in opacity and, finally, the onset of semiconvection. For the masses considered in Task3.2 and Task3.3, semiconvection appears very easily, as the mass of the convective core increases with time, leading to a quasi-discontinuity in the He abundance.

As for the convective envelope, the numerical treatment of the border of the convective regions is a key aspect of the convective core evolution. In Fig. 7 we plot the evolution of the convective regions in the central part of 1.2 $M_\odot$ models computed with CLES (left panel) and with CESAM (right panel). While CLES treatment of convective borders keeps convectively unstable shells separated from the convective core (grey region), it seems that CESAM tends to connect these shells to the central convective region. In fact, the envelope of the curve $M_{cc}$ vs. $X_c$ for CESAM2k MB model approximately coincides with the “semiconvection” region in CLES plot. As a consequence, a larger central mixed region in CESAM2k MB than in CLES leads to a longer main sequence phase, as seen in Fig. 1. In fact, the value of $M_{cc}$, just before it begins to decrease, is 6% and 12%, respectively for 1.2 and 1.3 $M_\odot$, larger for CESAM2k MB models than for CLES ones. On the other hand, the corresponding values for CESAM2k B are 2% and 10% larger than CLES ones.

4 Diffusion coefficient differences

The discrepancies we found between CESAM2k MP and CLES diffusion efficiency are in good agreement with the comparisons already published by TBL94. The large differences between CESAM2k B and CLES are instead rather unexpected. Both codes, in fact, derive the diffusion velocities by solving the Burgers’ equations, however, the values of friction coefficients appearing in those equations are different in CESAM2k B and CLES approaches. The resistance coefficients $K_{ij}$, which represent the effects of collisions between the particles i and j, are $K_{ij} = C_{ij} F_{ij}^{(11)}$ in CESAM2k B, and $K_{ij} = C_{ij} 2 \ln \Lambda_{ij}$ in CLES (TBL94). The term $C_{ij}$ is the same in both formulations and depends on the mass, charge and concentration of the particles i and j. The values of the quantity $F_{ij}^{(11)}$ are derived from the numerical fits of the collision integrals (Paquette et al., 1986), and the term $\ln \Lambda_{ij}$ is the Coulomb logarithm from Iben & MacDonald (1985). Furthermore, while TBL94 adopt for the heat flux terms $z_{ij}$, $z'_{ij}$ and $z''_{ij}$ their low density asymptotic values, CESAM2k B computes them by using the collision integrals from Paquette et al. (1986).

As shown in Thoul & Montalbán (2007), the assumptions done in TBL94 can lead, for the Task3.2 A model, to diffusion velocities between 6 and 20% larger than those that would be obtained by using the Paquette’s coefficients. To further clarify this point, we replaced in Burgers equations the coefficients used in CLES
with those used in CESAM2k B and we re-computed the models for Task3.2. The new evolution of He surface abundance is plotted in Fig. 8 (left panel, thick line) together with the curves obtained directly by CESAM2k B, standard CLES, and CESAM2k MP. We see that the approximation adopted in TBL94 implies a helium surface abundances slightly smaller than those that would be obtained by using the numerical fits by Paquette. The new CLES values are close to CESAM2k MP ones, but still quite far from CESAM2k B results.

Another important difference between CESAM and CLES diffusion routines is that, while CESAM follows separately each element inside Z and determine the ionization degree of all the species, the standard version of CLES adopts full ionization, and follows only four species: H, He, electrons and an “average” element Z with atomic mass 8, charge 17.84. To test the consequences of these approximations we computed the evolution of 1.2 $M_\odot$ with an updated version of CLES that computes the ionization degree, and allows to follow separately up to 22 elements. In Fig. 8 (right panel) we plot the evolution of the He surface abundance for calculations considering full ionization, and partial ionization for the eleven most relevant elements in Z. We can conclude that, at least for masses lower than or equal to 1.2 $M_\odot$ the effect of partial ionization on the He diffusion velocity is negligible.

Finally, we checked the effect of the time step by computing CLES evolution tracks with smaller and larger steps, but no significant effect was detected in the diffusion efficiency.

**Fig. 8.** Curves of the helium mass fraction in the convective envelope as a function of age for a 1.2$M_\odot$ evolution. Left panel: thick line corresponds to models computed by CLES with Paquette coefficients, and the other three curves corresponds to the results already shown in Fig. 2. Right panel: evolution of the helium mass fraction in the convective envelope for Task3.2 models computed by an updated version of CLES assuming: full ionization (dotted line), partial ionization of the “average” element Z (solid line) and partial ionization of eleven elements that diffuse separately (dashed line).
5 Conclusions

We compared models corresponding to Task3.1, Task3.2 and Task3.3 which were computed with three different implementations of microscopic diffusion. The largest discrepancy (∼40%) appears between codes that model diffusion velocities by solving the Burgers' equations (CESAM2k B and CLES). A detailed analysis showed that the approximations used in Thoul et al. 1994 for the friction coefficients are not at the origin of this discrepancy. Computations with partial ionization has also shown that for masses smaller or equal to 1.2M⊙, the full ionization assumption has no detectable effects. Therefore, we conclude that the difference between CLES and CESAM2k B results origins from the routine solving the Burgers' equation system.

Moreover, we showed that the effect of the different treatments of the convection borders can lead, when diffusion is included, to significant discrepancies (up to 12%) for the mass and radius of convective regions.

Acknowledgments

The authors thank HELAS for financial support. JM and ST are supported by Prodex 8 COROT (C90197)

References

Bahcall, J. N., Pinsonneault, M. H., and Basu, S.: 2001, Astrophys. J. 555, 990
Burgers, J. M.: 1969, Flow Equations for Composite Gases, New York: Academic Press, 1969
Lebreton, Y.: 2007, these proceedings, EAS Publication Series
Michaud, G. and Proffitt, C. R.: 1993, in W. W. Weiss and A. Baglin (eds.), ASP Conf. Ser. 40: IAU Colloq. 157: Inside the Stars, pp 246-259
Monteiro, M. K. J. P. F. G., Lebreton, Y., Montalban, J., Christensen-Dalsgaard, J., Castro, M., Degl'Innocenti, S., Moya, A., Roxburgh, I. W., and Scuflaire, R. et al.: 2006, in F. Favata, A. Baglin, and J. Lochard (eds.), ESA Publications Division, ESA SP; ESA Spec. Publ. 1306, pp 363–372
Morel, P.: 1997, Astron. Astrophys. Suppl. Ser. 124, 597
Paquette, C., Pelletier, C., Fontaine, G., and Michaud, G.: 1986, Astrophys. J., Suppl. Ser. 61, 177
Richard, O., Michaud, G., and Richer, J.: 2001, Astrophys. J. 558, 377
Scuflaire, R., Montalbán, J., Théado, S., Bourge, P.-O., Miglio, A., Godart, M., Thoul, A., and Noels, A.: 2007a, Astrophys. Space. Sci.
Scuflaire, R., Théado, S., Montalbán, J., Bourge, P.-O., Miglio, A., Godart, M., Thoul, A., and Noels, A.: 2007b, Astrophys. Space. Sci.
Thoul, A. A., Bahcall, J. N., and Loeb, A.: 1994, Astrophys. J. 421, 828
Thoul, A. A., and Montalbán, J.: 2007, these proceedings, EAS Publication Series