Numerical issues on the thermally pulsing AGB stars

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Abstract. A version of the stars stellar evolution code has been developed that uses a non-simultaneous solution of the equations of stellar structure and evolution. In all other respects it is identical to the normal, fully simultaneous version. It is therefore possible to test the effect that solving equations in a non-simultaneous fashion has on the solutions obtained. Two cases are investigated: a 5 M_⊙ and a 3 M_⊙ star, both of metallicity Z=0.02. Prior to the asymptotic giant branch, the models are almost identical. However once thermal pulses start, the two methods of solution yield diverging results with the non-simultaneous code predicting longer interpulse periods.

Key words. stars: evolution - stars: AGB - numerical methods

1. Introduction

Stellar evolution is based upon the solution of the equations of stellar structure, together with equation governing the mixing and burning of certain important isotopes. For a spherically symmetric star that is non-rotating, these equations are (see e.g. Kippenhahn & Weigert [1990]):

- The equation of hydrostatic equilibrium,
  \[ \frac{dP}{dm} = -\frac{Gm}{4\pi r^4}, \] (1)
  where \( P, r \) and \( m \) are pressure, radius and the mass contained within a spherical shell of radius \( r \) respectively.

- The equation of mass conservation,
  \[ \frac{dr}{dm} = \frac{1}{4\pi r^2 \rho}, \] (2)
  where \( \rho \) is density.

- The equation of energy generation,
  \[ \frac{dL}{dm} = \epsilon, \] (3)
  where \( L \) is luminosity and \( \epsilon \) is the energy generation rate including nuclear energy generation, energy from gravitational sources and energy losses from neutrino emission.

- The equation of energy transport, which may be expressed as
  \[ \frac{d \ln T}{dm} = -\nabla \frac{d \ln P}{dm} \] (4)
  where \( \nabla \) depends on whether the region of the star is radiative or convective.
Assuming mixing is treated as a diffusive process, the equation governing mixing and burning for each isotope $X_i$ is given by:

$$
\frac{d}{dt} \left( \frac{dX_i}{dm} \right) + R_i - S_i = 0 \tag{5}
$$

where $\sigma$ is the diffusion coefficient, $R_i$ is the rate at which the species $i$ is being burnt by nuclear reactions, and $S_i$ is the rate at which it is being produced by nuclear reactions (Eggleton 1972). While these equations may be common to all evolution codes, the method employed to solve them varies. Three possible ways in which current codes can solve these equations may be identified. Before describing these methods it is necessary to define some terminology. A timestep is defined as the act of moving from a model at time $t$ to one at time $t + \Delta t$. To produce a model at a new timestep it is necessary to make iterations on the solution. When the changes to the current solution are sufficiently small the model is said to have converged. Bearing in mind these definitions, three approaches to solving the equations may be defined: non-simultaneous, partially simultaneous and fully simultaneous.

The non-simultaneous approach involves converging a solution for the structure for a given timestep, then using this structure to calculate the mixing and burning for that timestep. Iterations are made separately on the structure and the chemistry (mixing and burning). Examples of codes that employ this method include those of Stancliffe et al. (2000) and Herwig (2000). The partially simultaneous approach involves solving for the structure equations for an iteration, then performing an iteration on the mixing/burning. One continues alternating between structure and chemistry iterations until the next timestep is converged. Such an approach is used in the Mount Stromlo Stellar Structure Program (MSSSP) employed by Karakas et al. (2002), for example. Finally, the fully simultaneous approach involves solving all the equations together at each individual iteration of each timestep. This is the method employed by Eggleton (1971) in the original development of the STARS code and continues to be used in its current incarnations.

Motivated by the discrepancies that are apparent in calculations of thermally pulsing asymptotic giant branch (TP-AGB) stars carried out using different codes (Lugaro et al. 2003, Stancliffe et al. 2004a), it is important to address the issue of whether there is any difference in adopting one of these methods of solution over any of the others. While it is thought that simultaneous solution will not influence the results of evolution calculations (Herwig 2005), the effects have not been tested until now.

2. Results

The stellar evolution code STARS, originally developed by Eggleton (1971) and most recently updated by Pols et al. (1993), was used in this study. Derivatives of the original Eggleton code are unique in that they are the only codes to solve the equation of stellar structure and evolution in a fully simultaneous manner.

One would expect that if any difference exists between the methods of solution, it is likely to be greatest between the non-simultaneous and the fully simultaneous approaches. Therefore a non-simultaneous version of the code STARS has been developed. To do this, use has been made of pair of subroutines designed to follow the evolution of minor isotopes (see Stancliffe et al. 2005, Stancliffe 2005 for further details). These routines take the structure computed by the main routines and use it to compute the burning and mixing of material which is energetically unimportant. Thus it is possible to convert the STARS code into a non-simultaneous code by removing the equations of burning and mixing from the main code and placing them in these subroutines.

To compare the differences between the two codes a 5 M$_\odot$ star of initial metallicity Z=0.02 was evolved from the pre-main sequence to the asymptotic giant branch without mass loss or convective overshooting using both simultaneous and non-simultaneous approaches. The initial model had 499 mesh points. Once second dredge-up was over, the

\footnote{Not all codes treat mixing in this way.}
models were remeshed with 1999 mesh points$^{2}$ and the AGB specific mesh spacing function of Stancliffe, Tout, & Pols (2004b) was employed in order to ensure proper spatial resolution of the important features of AGB stars.

Throughout the pre-main sequence, main-sequence and red giant branch the evolution computed by the two methods is indistinguishable. At core helium burning the non-simultaneous model displays a blue loop that extends toward the blue more than the simultaneous model but this deviation is less than a tenth of a percent and should not be considered significant.

As the asymptotic giant branch is ascended the simultaneous model grows a larger core than the non-simultaneous model. Prior to second dredge-up the simultaneous model has a hydrogen-exhausted core that is about 0.3% larger than the core of the non-simultaneous model. The simultaneous model then undergoes deeper second dredge-up than the non-simultaneous model, resulting in it having a core that is 0.6% lighter. This difference is about an order of magnitude smaller than the difference between the simultaneous model and the comparable model of Karakas et al. (2002), computed with a partially simultaneous code. It therefore seems unlikely that the differences in details such as the core mass at first thermal pulse is due to the method of solution.

At the beginning of the TP-AGB the two models retain their similarities for a few thermal pulses. A rapid divergence in behaviour then sets in. This is demonstrated in the evolution of the helium luminosities for both models as shown in Figure 1. The first three thermal pulses all have approximately similar peak helium luminosities. However, the interpulse period following the third thermal pulse is much longer in the non-simultaneous model. This then results in the fourth thermal pulse of that model being much stronger.

Fig. 1. Evolution of the helium luminosity as a function of age. The simultaneous model is shown as a solid line; the non-simultaneous model is the dashed line. Note that the non-simultaneous model has been shifted forward by 4.44 x 10$^4$ yr to make the first thermal pulses coincident.

How much of the deviation is due to the fact that the two models have slightly different core mass at the beginning of the TP-AGB? While the initial difference is minimal it is not inconceivable that a small difference in initial conditions can lead to a larger difference later in the evolution. To assess the impact of just the difference in the method of solution, a starting model for a run with the non-simultaneous code was taken from the simultaneous run, just after second dredge-up. The evolution of the helium luminosity compared to the simultaneous code evolution is shown in Figure 2. Again, the initial pulses are similar but are seen to diverge after a couple of pulses. It would be desirable to continue the sequence to compare the behaviour over a longer run of thermal pulses but a numerical instability that could not be overcome in the non-simultaneous run meant this could not be done.

It therefore seems that simultaneous and non-simultaneous methods of solution do not yield the same results.

2.1. 3 $M_\odot$ models

Having noted that the two solution methods give different results, it is important to test whether these results extended to lower masses. Therefore 3 $M_\odot$, Z=0.02 models were also produced using both codes. The details of

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2 This is twice the number normally employed and was used in case making the code non-simultaneous required additional spatial resolution.
Table 1. Details of the simultaneous 3 M⊙ model. The data are TP – the thermal pulse number, $M_H$ – the hydrogen free core mass, $\tau_p$ – the interpulse period, $L_{\text{He}}^\text{max}$ – the peak luminosity from helium burning, $\Delta M_H$ – the hydrogen free core mass growth during the interpulse, $\Delta M_{\text{DUP}}$ – the mass of material dredged up, $\lambda = \Delta M_{\text{DUP}}/\Delta M_H$ – the dredge-up efficiency and C/O – the surface carbon-to-oxygen ratio by number.

<table>
<thead>
<tr>
<th>TP</th>
<th>$M_H$ (M⊙)</th>
<th>$\tau_p$ (10^4 yr)</th>
<th>$\log (L_{\text{He}}^\text{max}/L_\odot)$</th>
<th>$\Delta M_H$ (M⊙)</th>
<th>$\Delta M_{\text{DUP}}$ (M⊙)</th>
<th>$\lambda$</th>
<th>C/O</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>0.55267</td>
<td>...</td>
<td>4.36792</td>
<td>0.01628</td>
<td>...</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.56894</td>
<td>7.60</td>
<td>6.27639</td>
<td>0.00440</td>
<td>...</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.57333</td>
<td>7.78</td>
<td>5.56767</td>
<td>0.00297</td>
<td>...</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.57629</td>
<td>8.89</td>
<td>6.65021</td>
<td>0.00580</td>
<td>...</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.58208</td>
<td>9.33</td>
<td>6.62750</td>
<td>0.00574</td>
<td>...</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.58781</td>
<td>8.81</td>
<td>6.80665</td>
<td>0.00621</td>
<td>0.00047</td>
<td>0.076</td>
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<tr>
<td>7</td>
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<td>8.22</td>
<td>6.90432</td>
<td>0.00633</td>
<td>0.00113</td>
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</tr>
<tr>
<td>8</td>
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<td>7.03324</td>
<td>0.00660</td>
<td>0.00190</td>
<td>0.288</td>
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</tr>
<tr>
<td>9</td>
<td>0.60345</td>
<td>7.50</td>
<td>7.16711</td>
<td>0.00701</td>
<td>0.00266</td>
<td>0.379</td>
<td>0.393</td>
</tr>
</tbody>
</table>

Table 2. Details of the non-simultaneous 3 M⊙ model. The headings are the same as in Table 1.

<table>
<thead>
<tr>
<th>TP</th>
<th>$M_H$ (M⊙)</th>
<th>$\tau_p$ (10^4 yr)</th>
<th>$\log (L_{\text{He}}^\text{max}/L_\odot)$</th>
<th>$\Delta M_H$ (M⊙)</th>
<th>$\Delta M_{\text{DUP}}$ (M⊙)</th>
<th>$\lambda$</th>
<th>C/O</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.54981</td>
<td>...</td>
<td>5.64095</td>
<td>0.01704</td>
<td>...</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.56684</td>
<td>6.87</td>
<td>5.33562</td>
<td>0.00241</td>
<td>...</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.56925</td>
<td>8.99</td>
<td>6.45104</td>
<td>0.00517</td>
<td>...</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.57441</td>
<td>10.99</td>
<td>6.65133</td>
<td>0.00591</td>
<td>...</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.58032</td>
<td>10.59</td>
<td>6.87245</td>
<td>0.00642</td>
<td>...</td>
<td>0.315</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.58666</td>
<td>10.01</td>
<td>6.96026</td>
<td>0.00663</td>
<td>0.00064</td>
<td>0.097</td>
<td>0.318</td>
</tr>
<tr>
<td>7</td>
<td>0.59265</td>
<td>9.52</td>
<td>7.12672</td>
<td>0.00707</td>
<td>0.00142</td>
<td>0.201</td>
<td>0.328</td>
</tr>
<tr>
<td>8</td>
<td>0.59830</td>
<td>9.17</td>
<td>7.28263</td>
<td>0.00755</td>
<td>0.00222</td>
<td>0.294</td>
<td>0.347</td>
</tr>
</tbody>
</table>

As with the 5 M⊙ models, the 3 M⊙ also display different behaviour, despite entering the TP-AGB with core masses within less than a percent of one another. The main difference again seems to be in the interpulse periods which are again larger in the case of the non-simultaneous code. The longer interpulse period also means that there is greater core growth in the non-simultaneous code. The non-simultaneous model also gives more violent thermal pulses. This is probably related to the longer interpulse period (see the discussion in Stancliffe et al. 2004b).

It terms of the onset of third dredge-up and its depth, both models give similar results. In both cases TDUP sets in when the H-exhausted core mass exceeds 0.585 M⊙ and this happens on the sixth pulse in both models. Over the few thermal pulses with TDUP both models give comparable dredge-up efficiencies, with the simultaneous code giving slightly lower efficiencies (which may be due to the slightly lower pulse strength). Curiously, while the simultaneous model gives slightly less TDUP its C/O ratio becomes higher than the non-simultaneous model.

3. Discussion

From the albeit limited example of the models presented above, it appears that the important quantities of the core mass at first thermal pulse...
The simultaneous model is shown as a solid line; the non-simultaneous model is the dashed line. This time both models have been given the same initial post-second dredge-up model.

and the core mass at which third dredge-up occurs are not affected substantially by the use of a simultaneous or non-simultaneous solution as they differ by less than a percent in both these runs. By contrast, the difference between the core mass at first thermal pulse in simultaneous run is around 7% smaller than the corresponding model of the partially simultaneous code of Karakas et al. (2002). This would suggest that the differences that occur between the predictions are not due to the method of solution used.

However, there are discrepancies between the predictions of the two methods. The non-simultaneous solution gives longer interpulse periods than the fully simultaneous solution. In the case of the 3 M$_\odot$ model, a deviation in the surface C/O ratio is also seen. The reasons for these deviations is unclear but they do point to the fact that it cannot be claimed that the fully simultaneous and non-simultaneous methods give identical results. The preliminary nature of this work means it is not yet possible to say whether these discrepancies may be important.

If the method of solution does not matter, is there any purpose in doing stellar evolution using a simultaneous code? It has already been noted that prior to the TP-AGB no differences are observed in the HR diagram. Are there any other phases of evolution where a simultaneous solution might be important?

Two possibilities spring to mind. First, there is the issue of very late thermal pulses (VLTPs) and the formation of born-again AGB stars. If a star leaves the TP-AGB at just the right point it will still have a reservoir of helium as it evolves down the white dwarf cooling track. As it does so the helium may reignite to give one last thermal pulse. Because the hydrogen burning shell is no longer burning the intershell convection zone is no longer trapped by an entropy barrier as it would be on the TP-AGB. This enables hydrogen to be engulfed in the pocket which can lead to the formation of hydrogen-deficient post-AGB objects. This scenario is believed to explain the evolution of objects like FG Sag and Sakurai’s Object (Hajduk et al. 2005).

In such a situation the mixing, burning and structure are intimately linked and one might reasonably expect that a simultaneous solution may be necessary to obtain the correct answer. Unfortunately, the VLTP scenario is an extremely numerically demanding phase of evolution and the author has not yet been able to produce a model for this phase using the stars code.

The phenomenon of hot TDUP, described in detail by Herwig (2004), (but seen earlier, though not described as such, in the work of Chieh et al. 2001) might also require simultaneous solution. Found to occur in low metallicity stars, hot TDUP occurs when the temperature at the base of the convective envelope during TDUP is sufficiently hot for H-burning via the CNO cycle to take place. This results in the dredging up of both carbon and nitrogen. The occurrence of hot TDUP can lead to extreme amounts of dredge-up with the envelope eating its way through the entire intershell (Herwig 2004)!

Unfortunately for the exponents of the use of a simultaneous solution, it seems that calculations yield similar results to those from a non-simultaneous code. Figure 3 shows the evolution of the H- and He-exhausted cores of a 5 M$_\odot$ model of metallicity Z=10$^{-4}$. The dredge-up rapidly becomes very deep, extending right the way through the intershell. This is
4. Conclusions

For the first time the effects of using a fully simultaneous method of solution of the equations of stellar structure and evolution have been tested. It is found that prior to the TP-AGB the results of a simultaneous solution are virtually indistinguishable from those computed using a non-simultaneous method, as expected. However, as the evolution is followed along the TP-AGB, divergence is seen to occur between the two methods. The non-simultaneous method seems to give longer interpulse periods. However, important quantities like the core mass at first thermal pulse and the core mass at which TDUP begins as computed by the two different methods are the same to within a percent. This contrasts with the discrepancy of as much as 7% seen between results from different evolution codes. It therefore seems unlikely that the method of solution is responsible for the differences seen between calculations made using different evolution codes.

There does exist a difference in behaviour between models computed with non-simultaneous and fully simultaneous methods of solution. The reason for this divergence in behaviour is not understood and further work needs to be done to explain why this occurs. There may exist some phases of evolution where a fully simultaneous solution is necessary to obtain the correct behaviour.

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References

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