Week 8

We have now derived all of the equations necessary for constructing a model of a star. In this lecture we will consider in detail how a stellar model is actually constructed by computing a numerical solution to the equations of stellar structure.

1 Numerical calculation of stellar models

One almost always considers the evolution of a star of a given mass. Hence it is convenient to rewrite the equations of stellar structure with the mass $m = m(r)$ as the independent variable. This may be done by noting that for any quantity ϕ we can write

$$\frac{d\phi}{dm} = \frac{d\phi}{dr}\frac{dr}{dm} = \frac{1}{4\pi\rho r^2}\frac{d\phi}{dr}. \tag{1}$$

By transforming the equations of stellar structure that we have derived

$$\begin{aligned}
\frac{dm}{dr} &= 4\pi r^2\rho \\
\frac{dP}{dr} &= -\frac{Gm}{r^2}\rho \\
\frac{dL}{dm} &= \epsilon \\
\frac{dT}{dr} &= -\frac{3\kappa\rho L(r)}{16\pi acr^2T^3} \quad \text{radiative energy transport} \\
\frac{dT}{dr} &= \frac{\gamma-1}{\gamma}\frac{P}{T}\frac{dP}{dr} \quad \text{convective energy transport}
\end{aligned} \tag{2}$$

we obtain

$$\begin{aligned}
\frac{dr}{dm} &= \frac{1}{4\pi r^2\rho} \\
\frac{dP}{dm} &= -\frac{Gm}{4\pi r^4} \\
\frac{dL}{dm} &= \epsilon \\
\frac{dT}{dm} &= -\frac{3\kappa}{4acT^3}\frac{L}{16\pi^2r^4} \quad \text{radiative energy transport} \\
\frac{dT}{dm} &= \frac{\gamma-1}{\gamma}\frac{T}{P}\frac{dP}{dm} \quad \text{convective energy transport.}
\end{aligned} \tag{3}$$

These equations must be supplemented by expressions for ρ, γ, κ and ϵ as functions of P and T, and the chemical composition. As we have seen, these expressions are obtained from thermodynamics, atomic physics and nuclear physics.

1.1 Boundary conditions at the centre

The differential equations (3) must be supplemented by suitable boundary conditions. At the stellar centre, we have

$$r = 0 \ \text{ and } \ L = 0 \ \text{ for } \ m = 0. \tag{4}$$

1.2 Boundary conditions at the surface

The surface boundary conditions involve specifying values of T and P at the surface of the model. We can choose the point where $T = T_{\rm eff}$ as the surface of the model. As we will see below, this location is known as the *photosphere*, and is the region from which most of the radiation from the star propagates

out into free space. Once we have specified the temperature boundary condition, we need to find the appropriate value of the pressure at this temperature.

In the stellar atmosphere, the photons are radiated directly into space, without being substantially absorbed, and hence the transport of energy does not require a large temperature gradient, so the energy can be transported by radiation and will not be transported by convection. The optical properties of the atmosphere are usually described in terms of the so-called *optical depth*, defined as

$$\tau = \int_r^\infty \kappa\rho dr. \tag{5}$$

Since $\kappa\rho = 1/\lambda_{\rm ph}$, where $\lambda_{\rm ph}$ is the mean free path of the photon (see lecture of week 6), a photon can be radiated directly to space from layers which have an optical depth of about 1 (or smaller), since this optical depth corresponds to a length scale $dr \sim \lambda_{\rm ph}$.

Rewriting eqn. (2) for the diffusive flux of radiative energy, F, as

$$\frac{dT^4}{dr} = -\frac{3F}{ac}\kappa\rho = \frac{3F}{ac}\frac{d\tau}{dr} \tag{6}$$

(note the sign change because τ decreases with r) we have

$$T^4 = \frac{3F}{ac}(\tau + \text{constant}), \tag{7}$$

since the thin atmosphere can be considered a plane parallel layer with $dF/dr \approx 0$ (i.e through which the radiative flux is approximately constant).

Of course, the eqns. (6) and (7) become invalid when one approaches the very optically thin layers high in the atmosphere. Because of the deceasing density, the mean free path of the photons there will become comparable to, and eventually larger than, the distance which is left for the photons to reach free space. Hence the whole diffusion approximation breaks down, and one has to solve the far more complicated full set of radiation transport equations in the stellar atmosphere.

We can employ eqn. (7) in the lower atmosphere, where the diffusion approximation become relevant, but we need the value of the constant of integration which appears in this equation. The theory of stellar atmospheres suggests the value of 2/3 as a simple approximation for this constant, and hence we obtain

$$T^4 = \frac{3F}{ac}\left(\tau + \frac{2}{3}\right). \tag{8}$$

We note that the Stefan-Boltzmann constant is given by

$$\sigma = \frac{ac}{4}, \tag{9}$$

and the Stefan-Boltzmann law gives

$$F = \sigma T_{\rm eff}^4 = \frac{ac}{4}T_{\rm eff}^4. \tag{10}$$

Hence, substituting for the flux from eqn. (10) into eqn. (8) gives

$$T^4 = \frac{3}{4}T_{\rm eff}^4\left(\tau + \frac{2}{3}\right), \tag{11}$$

which shows that $T = T_{\rm eff}$ when $\tau = 2/3$. This level in the atmosphere is known as the *photosphere*. It is the level from which the bulk of the radiation is emitted into space, and we can adopt it as the location of the outer boundary for our stellar models.

To evaluate the photospheric value of pressure, and hence the pressure at our outer boundary condition, we define a mean opacity $\langle\kappa\rangle$, averaged over the stellar atmosphere above the photospheric radius, $R_{\rm ph}$, through the relation

$$\tau_{\rm ph} = \frac{2}{3} = \langle\kappa\rangle\int_{R_{\rm ph}}^\infty \rho dr. \tag{12}$$

We now approximate the gravitational acceleration in the atmosphere by a constant value $GM/R_{\rm ph}^2$, and obtain

$$P_{\rm ph} = \int_{R_{\rm ph}}^{\infty} \frac{GM}{R_{\rm ph}^2} \rho dr = \frac{2}{3\langle\kappa\rangle} \frac{GM}{R_{\rm ph}^2}. \tag{13}$$

Together with $L = 4\pi R^2 \sigma T^4$, this is the required surface boundary condition, applied at $T = T_{\rm eff}$. More accurate surface boundary conditions, which are implemented in modern numerical computations, can be formulated by fitting the stellar model solution outlined above onto the solution for a stellar atmosphere.

As an example of stellar models that have been computed, Fig. 1.2 shows the location of the main sequence stars of uniform chemical composition (the so-called zero-age main sequence) on a theoretical H-R diagram.

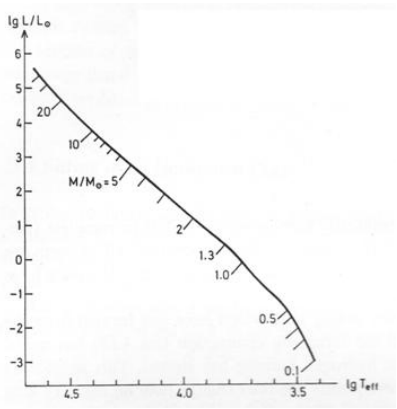

Figure 1: H-R diagram of the zero-age main sequence for composition $X = 0.685$ and $Y = 0.294$. The location of several models with masses between 0.1 and 22 solar masses are indicated (from Kippenhahn & Weigert 1990, Stellar Structure & Evolution, Springer-Verlag).

1.3 Midpoint fitting method

We now consider in some detail the practical problem of actually calculating a stellar model numerically. In week 4 we considered how to construct numerical solutions to the Lane-Emden equation that governs the structure of polytropic stellar models, and we adopt a similar procedure here. Our approach will deviate from that presented in week 4 because the four equations of stellar structure are supplemented by boundary conditions at both the centre and the surface of the star, and this complicates the process of obtaining a numerical solution. When solving the Lane-Emden equation we had two boundary conditions defined at the centre of the star, and this allowed us to develop approximate expressions for the Lane-Emden equation that could be solved numerically by stepping out from the centre of the star, using the boundary conditions as initial conditions for our integration, until we reached the surface of the model. When solving the equations of stellar structure, because we need to satisfy boundary conditions at the centre and the surface, we will integrate outwards from the centre of the star, and inwards from the surface, and try to match the solutions at the half-way point. In general, the outward and inward integrations will not meet in the middle, and the matching procedure requires repeated integrations to be undertaken with adjustment of a subset of the boundary conditions until the solutions match at the mid-point to a specified level of accuracy.

1.3.1 Difference equations

We will now develop approximations to the stellar structure equations (3) that allow us to integrate outwards from the centre of a stellar model and inwards from the surface. Consider a star of mass M_* that is discretised into N integration points and $N-1$ mass shells. The innermost integration point is located at the stellar centre, where the mass and radius are defined to be zero ($m = r = 0$) and the outermost one is located at the stellar surface where the mass is equal to the stellar mass M_*. Hence we can write

$$M_* = \sum_{i=1}^{N-1} \Delta m_i \tag{14}$$

where we use the index i to reference the integration points and the mass shells, and the mass contained in each mass shell is denoted Δm_i. Note that $i = 0$ represents the innermost integration point located at the centre where the mass $m_{i=0} = 0$. For a general integration point i, the interior mass can be written

$$m_i = \sum_{j=1}^{i} \Delta m_j. \tag{15}$$

From now on we will assume that the mass shells all have the same mass, Δm. We can approximate the derivatives of quantities such as the pressure, P, using finite difference approximations

$$\frac{dP}{dm} \approx \frac{\Delta P}{\Delta m} = \frac{P_{i+1} - P_i}{m_{i+1} - m_i}, \tag{16}$$

where P_i, $P_{\rm i+1}$, m_i and m_{i+1} are the pressures and interior masses defined at the arbitrary integration points i and $i + 1$. Using the notation $\Delta m = m_{i+1} - m_i$, the equations of stellar structure can be approximated as

$$\begin{aligned}
\frac{r_{i+1} - r_i}{\Delta m} &= \frac{1}{4\pi r_i^2 \rho_i} \\
\frac{P_{i+1} - P_i}{\Delta m} &= -\frac{G m_i}{4\pi r_i^4} \\
\frac{L_{i+1} - L_i}{\Delta m} &= \epsilon_i \\
\frac{T_{i+1} - T_i}{\Delta m} &= -\frac{3\kappa_i}{4acT_i^3}\frac{L_i}{16\pi^2 r_i^4} && \text{radiative energy transport} \\
\frac{T_{i+1} - T_i}{\Delta m} &= \frac{\gamma - 1}{\gamma}\frac{T_i}{P_i}\frac{P_{i+1} - P_i}{\Delta m} && \text{convective energy transport}
\end{aligned} \tag{17}$$

and hence we obtain equations that allow us to integrate out from the centre of the star

$$\begin{aligned}
r_{i+1} &= r_i + \Delta m \times \frac{1}{4\pi r_i^2 \rho_i} \\
P_{i+1} &= P_i - \Delta m \times \frac{G m_i}{4\pi r_i^4} \\
L_{i+1} &= L_i + \Delta m \times \epsilon_i \\
T_{i+1} &= T_i - \Delta m \times \frac{3\kappa_i}{4acT_i^3}\frac{L_i}{16\pi^2 r_i^4} && \text{radiative energy transport} \\
T_{i+1} &= T_i + \Delta m \times \frac{\gamma - 1}{\gamma}\frac{T_i}{P_i}\frac{P_{i+1} - P_i}{\Delta m} && \text{convective energy transport.}
\end{aligned} \tag{18}$$

Equations (18) are supplemented by the boundary conditions $r_i = 0$ and $L_i = 0$ for the innermost integration point $i = 0$ (but see below for a more detailed discussion about boundary conditions). To start the integration, it is also clear from inspection of eqns. (18) that we need to specify values for $T_{i=0} = T_{\rm c}$ and $P_{i=0} = P_{\rm c}$. As we will see below, the mid-point fitting algorithm will consist of integrating outwards from the centre repeatedly, adjusting the values of $T_{\rm c}$ and $P_{\rm c}$, until the solutions obtained from the outwards and inwards integrations agree with one another at the mid-point.

We now consider the equations to be used to integrate inwards from the surface. We can write

approximations to the stellar structure eqns. (18) in the form

$$\begin{aligned}
\frac{r_i - r_{i-1}}{\Delta m} &= \frac{1}{4\pi r_i^2 \rho_i} \\
\frac{P_i - P_{i-1}}{\Delta m} &= -\frac{G m_i}{4\pi r_i^4} \\
\frac{L_i - L_{i-1}}{\Delta m} &= \epsilon_i \\
\frac{T_i - T_{i-1}}{\Delta m} &= -\frac{3\kappa_i}{4acT_i^3}\frac{L_i}{16\pi^2 r_i^4} \qquad \text{radiative energy transport} \\
\frac{T_i - T_{i-1}}{\Delta m} &= \frac{\gamma - 1}{\gamma}\frac{T_i}{P_i}\frac{P_i - P_{i-1}}{\Delta m} \qquad \text{convective energy transport}
\end{aligned} \tag{19}$$

and hence we obtain equations that allow us to integrate out from the surface of the star

$$\begin{aligned}
r_{i-1} &= r_i - \Delta m \times \frac{1}{4\pi r_i^2 \rho_i} \\
P_{i-1} &= P_i + \Delta m \times \frac{G m_i}{4\pi r_i^4} \\
L_{i-1} &= L_i - \Delta m \times \epsilon_i \\
T_{i-1} &= T_i + \Delta m \times \frac{3\kappa_i}{4acT_i^3}\frac{L_i}{16\pi^2 r_i^4} \qquad \text{radiative energy transport} \\
T_{i-1} &= T_i - \Delta m \times \frac{\gamma - 1}{\gamma}\frac{T_i}{P_i}\frac{P_i - P_{i-1}}{\Delta m} \qquad \text{convective energy transport.}
\end{aligned} \tag{20}$$

Equations (20) are supplemented by the boundary conditions $T_{N-1} = T_{\rm s}$ and $P_{N-1} = P_{\rm s}$, where $T_{\rm s}$ and $P_{\rm s}$ are the temperature and pressure at the surface of the model. As can be seen from inspection of eqns. (20), we also require boundary conditions to be specified for $r_{N-1} = R_{\rm s}$ and $L_{N-1} = L_{\rm s}$, the surface values for the radius and luminosity, in order to be able to start the inwards integration from the surface. As will be discussed below, a key element of the mid-point fitting procedure will be to integrate inwards repeatedly from the surface, adjusting the values of $R_{\rm s}$ and $L_{\rm s}$, while keeping $T_{\rm s}$ and $P_{\rm s}$ fixed, until the solutions obtained from the inwards and outwards integrations meet at the midpoint.

Note also that we have expressions for ϵ_i and κ_i in terms of the density ρ_i and temperature T_i. We obtain the density from the equation of state

$$\rho_i = \frac{\mu m_H P_i}{k_{\rm B} T_i} \tag{21}$$

and then use Kramers opacity

$$\kappa_i = \kappa_0 \rho_i T_I^{-7/2} \tag{22}$$

and the energy generation rate

$$\epsilon_i = \epsilon_{\rm pp} \rho_i T_i^{\alpha} + \epsilon_{\rm CNO} \rho_i T_i^{\beta} \tag{23}$$

where κ_0, $\epsilon_{\rm pp}$ and $\epsilon_{\rm CNO}$ are constants that define the magnitudes of the Kramers opacity and energy generation rate per unit mass from the PP-chain and CNO-cycle, respectively.

1.3.2 A closer look at the boundary conditions

It is obvious from inspection of eqns. (17) and (18) that these equations cannot be applied to a situation where the integration is initiated at the very centre of a star where $m = r = 0$, since we have factors of r_i in the denominator. Hence, in practice we must start the integration at some small distance from the centre such that $r_{i=0} > 0$ and $m_{i=0} > 0$. Formally, this then requires a change in the boundary conditions because the values at the centre of the star do not apply at the location of the first integration point. Using the stellar structure eqns. (3), we can obtain approximate values to be specified at the first integration point.

From the equation of mass conservation we have

$$dr = \frac{dm}{4\pi r^2 \rho}. \tag{24}$$

Assuming that very close to the centre that $\rho = \rho_{\rm c}$, and applying the boundary condition $r = 0$ at $m = 0$, we have

$$\int_0^r r^2 dr \approx \int_0^m \frac{1}{4\pi\rho_{\rm c}} dm \implies \frac{r^3}{3} = \frac{m}{3\pi\rho_{\rm c}}. \tag{25}$$

Hence, if our first integration point is placed at a small distance from the centre of the stellar model, then the radius and mass at that point are related by

$$r_{i=0} = \left(\frac{3m_{i=0}}{4\pi\rho_{\rm c}}\right)^{1/3}. \tag{26}$$

Similarly, if the gradient in energy sources is not too large, then close to the centre of the star we can write

$$\int_0^L dL \approx \epsilon \int_0^m dm \implies L = \epsilon(\rho_{\rm c}, T_{\rm c}) m. \tag{27}$$

Applying this to our numerical scheme gives a boundary condition for L at the innermost integration point

$$L_{i=0} = \epsilon(\rho_{\rm c}, T_{\rm c}) m_{i=0}. \tag{28}$$

We assume that the star is in hydrostatic equilibrium, and that the density near the centre can be approximated $\rho = \rho_{\rm c}$. This gives

$$r \approx \left(\frac{3m}{4\pi\rho_{\rm c}}\right)^{1/3} \tag{29}$$

and

$$\frac{dP}{dm} = -\frac{Gm}{4\pi r^4} \implies \int_{P_{\rm c}}^P dP \approx \int_0^m -\frac{Gm}{4\pi}\left(\frac{4\pi\rho_{\rm c}}{3m}\right)^{4/3} dm. \tag{30}$$

Integrating we obtain

$$P - P_{\rm c} = -\frac{3G}{8\pi}\left(\frac{4\pi\rho_{\rm c}}{3}\right)^{4/3} m^{2/3}. \tag{31}$$

Hence, the pressure boundary condition at our innermost integration point becomes

$$P_{i=0} = P_{\rm c} - \frac{3G}{8\pi}\left(\frac{4\pi\rho_{\rm c}}{3}\right)^{4/3} m_{i=0}^{2/3}. \tag{32}$$

In the case of radiative energy transport we have

$$\frac{dT}{dm} = -\frac{3\kappa L}{64\pi^2 a c r^4 T^3} \approx -\frac{3\kappa\epsilon_{\rm c} m}{64\pi^2 a c T^3}\left(\frac{4\pi\rho_{\rm c}}{3m}\right)^{4/3}. \tag{33}$$

Integrating yields

$$\int_{T_{\rm c}}^T T^3 dT = -\frac{\kappa_{\rm c}\epsilon_{\rm c}}{16\pi a c}\left(\frac{4\pi\rho_{\rm c}^4}{3}\right)^{1/3} \int_0^m m^{-1/3} dm \tag{34}$$

which evaluates to

$$T^4 - T_{\rm c}^4 = -\frac{\kappa_{\rm c}\epsilon_{\rm c}}{2ac}\left(\frac{3\rho_{\rm c}^2}{4\pi}\right)^{2/3} m^{2/3}. \tag{35}$$

Hence the temperature boundary condition at the innermost integration point becomes

$$T_{i=0}^4 = T_{\rm c}^4 - \frac{\kappa_{\rm c}\epsilon_{\rm c}}{2ac}\left(\frac{3\rho_{\rm c}^2}{4\pi}\right)^{2/3} m_{i=0}^{2/3}, \tag{36}$$

where $\kappa_{\rm c}$ and $\epsilon_{\rm c}$ indicate that the opacity and energy generation rates are calculated using the central values $\rho_{\rm c}$ and $T_{\rm c}$. Similarly a temperature boundary condition can be obtained using the adiabatic temperature gradient if the central regions are expected to be fully convective, as may occur in high mass stars. Obtaining this is left as an exercise.

1.3.3 Iterating the solutions to convergence

Consider the situation where we have developed a computer code to solve the equations of stellar structure based on eqns. (18) and (20), we have applied the boundary conditions at the inner and outer integration points, and we have run the code so that it integrates the solution from the centre to the integration point that lies at the midpoint, and it integrates the solution from the surface to the same midpoint. Unless we have been exceptionally fortunate, the guesses that we have made for the boundary condition values of $T_{\rm c}$, $P_{\rm c}$, $R_{\rm s}$ and $L_{\rm s}$ will lead to solutions that do not meet at the midpoint. In other words, the values of P, T, r and L at the midpoint obtained for the outward integration will not be equal to those obtained from the inward integration. A stellar model can only be said to have been successfully computed when all of these values agree (at least to within some specified tolerance). A satisfactory solution can be obtained by repeatedly adjusting the values of $T_{\rm c}$, $P_{\rm c}$, $R_{\rm s}$ and $L_{\rm s}$ and running the integrations until they meet in the middle. The question is, what is the best strategy for doing this? Guess work? Never a good idea! Choosing all possible reasonable values of $T_{\rm c}$, $P_{\rm c}$, $R_{\rm s}$ and $L_{\rm s}$ and repeating the calculations until the best set of choices is hit upon? That will in general be too expensive in terms of computing time given that the range of possible values is enormous. Fortunately, there is a more sophisticated and computationally efficient approach available to us.

First, let us remind ourselves that the outwards and inwards integrations will yield values for r, P, T and L throughout the star. Let us define the difference between the values of r at the midpoint obtained from the outwards and inwards integrations as $r_{\rm diff} = r_{\rm outwards} - r_{\rm inwards}$. Let us also define the differences in the values of P, T and L in the same way:

$$\begin{aligned} P_{\rm diff} &= P_{\rm outwards} - P_{\rm inwards} \\ T_{\rm diff} &= T_{\rm outwards} - T_{\rm inwards} \\ L_{\rm diff} &= L_{\rm outwards} - L_{\rm inwards}. \end{aligned} \tag{37}$$

Now suppose we change the central pressure in the computer code, so that $P_{\rm c} \rightarrow P_{\rm c} + \delta P_{\rm c}$, where $\delta P_{\rm c}$ is some small positive change in $P_{\rm c}$, and we rerun the calculation, keeping all the other boundary conditions equal to their original values. This will change the solution produced by the outwards integration, and we will obtain new values of $r_{\rm diff}$, $P_{\rm diff}$, $T_{\rm diff}$ and $L_{\rm diff}$. Let us use the notation $(\delta r_{\rm diff})_{\rm P}$ to denote the change in $r_{\rm diff}$ that arises when we change the value of $P_{\rm c}$ by an amount $\delta P_{\rm c}$. We also denote the change in $P_{\rm diff}$ that arises by $(\delta P_{\rm diff})_{\rm P}$, and similarly for the changes in $T_{\rm diff}$ and $L_{\rm diff}$ we define $(\delta T_{\rm diff})_{\rm P}$ and $(\delta L_{\rm diff})_{\rm P}$. Note that the values of $(\delta r_{\rm diff})_{\rm P}$ etc correspond to subtracting the new value of $r_{\rm diff}$ from the old value. This point is important as it defines the signs of $(\delta r_{\rm diff})_{\rm P}$ etc.

Now let us also run the code with a small change in the value of $T_{\rm c} \rightarrow T_{\rm c} + \delta T_{\rm c}$, with the other boundary conditions having their original values. This will give rise to changes in $r_{\rm diff}$, $P_{\rm diff}$, $T_{\rm diff}$ and $L_{\rm diff}$. We will denote these changes as $(\delta r_{\rm diff})_{\rm T}$, $(\delta P_{\rm diff})_{\rm T}$, $(\delta T_{\rm diff})_{\rm T}$ and $(\delta L_{\rm diff})_{\rm T}$. Repeating this procedure with small changes to $R_{\rm s}$ and $L_{\rm s}$ will give rise to changes in $r_{\rm diff}$, $P_{\rm diff}$, $T_{\rm diff}$ and $L_{\rm diff}$ that we will denote as $(\delta r_{\rm diff})_{\rm R}$, $(\delta P_{\rm diff})_{\rm R}$, $(\delta T_{\rm diff})_{\rm R}$, $(\delta L_{\rm diff})_{\rm R}$ and $(\delta r_{\rm diff})_{\rm L}$, $(\delta P_{\rm diff})_{\rm L}$, $(\delta T_{\rm diff})_{\rm L}$, $(\delta L_{\rm diff})_{\rm L}$.

Now, it is clear that for small changes to the boundary condition values denoted by $\delta P_{\rm c}$, $\delta T_{\rm c}$, $\delta R_{\rm s}$ and $\delta L_{\rm s}$, we can write

$$\begin{aligned}
&\frac{(\delta r_{\rm diff})_{\rm P}}{\delta P_{\rm c}} \approx \frac{\partial r_{\rm diff}}{\partial P_{\rm c}}, \quad \frac{(\delta P_{\rm diff})_{\rm P}}{\delta P_{\rm c}} \approx \frac{\partial P_{\rm diff}}{\partial P_{\rm c}}, \quad \frac{(\delta T_{\rm diff})_{\rm P}}{\delta P_{\rm c}} \approx \frac{\partial T_{\rm diff}}{\partial P_{\rm c}}, \quad \frac{(\delta L_{\rm diff})_{\rm P}}{\delta P_{\rm c}} \approx \frac{\partial L_{\rm diff}}{\partial P_{\rm c}} \\
&\frac{(\delta r_{\rm diff})_{\rm T}}{\delta T_{\rm c}} \approx \frac{\partial r_{\rm diff}}{\partial T_{\rm c}}, \quad \frac{(\delta P_{\rm diff})_{\rm T}}{\delta T_{\rm c}} \approx \frac{\partial P_{\rm diff}}{\partial T_{\rm c}}, \quad \frac{(\delta T_{\rm diff})_{\rm T}}{\delta T_{\rm c}} \approx \frac{\partial T_{\rm diff}}{\partial T_{\rm c}}, \quad \frac{(\delta L_{\rm diff})_{\rm T}}{\delta T_{\rm c}} \approx \frac{\partial L_{\rm diff}}{\partial T_{\rm c}} \\
&\frac{(\delta r_{\rm diff})_{\rm R}}{\delta R_{\rm s}} \approx \frac{\partial r_{\rm diff}}{\partial R_{\rm s}}, \quad \frac{(\delta P_{\rm diff})_{\rm R}}{\delta R_{\rm s}} \approx \frac{\partial P_{\rm diff}}{\partial R_{\rm s}}, \quad \frac{(\delta T_{\rm diff})_{\rm R}}{\delta R_{\rm s}} \approx \frac{\partial T_{\rm diff}}{\partial R_{\rm s}}, \quad \frac{(\delta L_{\rm diff})_{\rm R}}{\delta R_{\rm s}} \approx \frac{\partial L_{\rm diff}}{\partial R_{\rm s}} \\
&\frac{(\delta r_{\rm diff})_{\rm L}}{\delta L_{\rm s}} \approx \frac{\partial r_{\rm diff}}{\partial L_{\rm s}}, \quad \frac{(\delta P_{\rm diff})_{\rm L}}{\delta L_{\rm s}} \approx \frac{\partial P_{\rm diff}}{\partial L_{\rm s}}, \quad \frac{(\delta T_{\rm diff})_{\rm L}}{\delta L_{\rm s}} \approx \frac{\partial T_{\rm diff}}{\partial L_{\rm s}}, \quad \frac{(\delta L_{\rm diff})_{\rm L}}{\delta L_{\rm s}} \approx \frac{\partial L_{\rm diff}}{\partial L_{\rm s}}
\end{aligned} \tag{38}$$

Hence, we can use the expressions in eqn. (38) to obtain expressions for how large a change in $r_{\rm diff}$,

$P_{\rm diff}$, $T_{\rm diff}$ and $L_{\rm diff}$ will result from imposed changes to the boundary condition values

$$\begin{aligned}
\left(\frac{\partial r_{\rm diff}}{\partial P_{\rm c}}\right)\Delta P_{\rm c} + \left(\frac{\partial r_{\rm diff}}{\partial T_{\rm c}}\right)\Delta T_{\rm c} + \left(\frac{\partial r_{\rm diff}}{\partial R_{\rm s}}\right)\Delta R_{\rm s} + \left(\frac{\partial r_{\rm diff}}{\partial L_{\rm s}}\right)\Delta L_{\rm s} &= \Delta r_{\rm diff} \\
\left(\frac{\partial P_{\rm diff}}{\partial P_{\rm c}}\right)\Delta P_{\rm c} + \left(\frac{\partial P_{\rm diff}}{\partial T_{\rm c}}\right)\Delta T_{\rm c} + \left(\frac{\partial P_{\rm diff}}{\partial R_{\rm s}}\right)\Delta R_{\rm s} + \left(\frac{\partial P_{\rm diff}}{\partial L_{\rm s}}\right)\Delta L_{\rm s} &= \Delta P_{\rm diff} \\
\left(\frac{\partial T_{\rm diff}}{\partial P_{\rm c}}\right)\Delta P_{\rm c} + \left(\frac{\partial T_{\rm diff}}{\partial T_{\rm c}}\right)\Delta T_{\rm c} + \left(\frac{\partial T_{\rm diff}}{\partial R_{\rm s}}\right)\Delta R_{\rm s} + \left(\frac{\partial T_{\rm diff}}{\partial L_{\rm s}}\right)\Delta L_{\rm s} &= \Delta T_{\rm diff} \\
\left(\frac{\partial L_{\rm diff}}{\partial P_{\rm c}}\right)\Delta P_{\rm c} + \left(\frac{\partial L_{\rm diff}}{\partial T_{\rm c}}\right)\Delta T_{\rm c} + \left(\frac{\partial L_{\rm diff}}{\partial R_{\rm s}}\right)\Delta R_{\rm s} + \left(\frac{\partial L_{\rm diff}}{\partial L_{\rm s}}\right)\Delta L_{\rm s} &= \Delta L_{\rm diff}
\end{aligned} \tag{39}$$

where $\Delta P_{\rm c}$, $\Delta T_{\rm c}$, $\Delta R_{\rm s}$, $\Delta L_{\rm s}$ represent the changes in the boundary condition values. The set of simultaneous equations in (39) can be expressed in matrix form

$$\begin{bmatrix}
\left(\frac{\partial r_{\rm diff}}{\partial P_{\rm c}}\right) & \left(\frac{\partial r_{\rm diff}}{\partial T_{\rm c}}\right) & \left(\frac{\partial r_{\rm diff}}{\partial R_{\rm s}}\right) & \left(\frac{\partial r_{\rm diff}}{\partial L_{\rm s}}\right) \\
\left(\frac{\partial P_{\rm diff}}{\partial P_{\rm c}}\right) & \left(\frac{\partial P_{\rm diff}}{\partial T_{\rm c}}\right) & \left(\frac{\partial P_{\rm diff}}{\partial R_{\rm s}}\right) & \left(\frac{\partial P_{\rm diff}}{\partial L_{\rm s}}\right) \\
\left(\frac{\partial T_{\rm diff}}{\partial P_{\rm c}}\right) & \left(\frac{\partial T_{\rm diff}}{\partial T_{\rm c}}\right) & \left(\frac{\partial T_{\rm diff}}{\partial R_{\rm s}}\right) & \left(\frac{\partial T_{\rm diff}}{\partial L_{\rm s}}\right) \\
\left(\frac{\partial L_{\rm diff}}{\partial P_{\rm c}}\right) & \left(\frac{\partial L_{\rm diff}}{\partial T_{\rm c}}\right) & \left(\frac{\partial L_{\rm diff}}{\partial R_{\rm s}}\right) & \left(\frac{\partial L_{\rm diff}}{\partial L_{\rm s}}\right)
\end{bmatrix}
\begin{bmatrix} \Delta P_{\rm c} \\ \Delta T_{\rm c} \\ \Delta R_{\rm s} \\ \Delta L_{\rm s} \end{bmatrix} =
\begin{bmatrix} \Delta r_{\rm diff} \\ \Delta P_{\rm diff} \\ \Delta T_{\rm diff} \\ \Delta L_{\rm diff} \end{bmatrix} \tag{40}$$

What we really want are the values of $\Delta P_{\rm c}$, $\Delta T_{\rm c}$, $\Delta R_{\rm s}$ and $\Delta L_{\rm s}$ that are required to give the desired/specified changes in $\Delta r_{\rm diff}$, $\Delta P_{\rm diff}$, $\Delta T_{\rm diff}$ and $\Delta L_{\rm diff}$, so that the solutions from the outwards and inwards integrations will agree at the midpoint. Writing the above matrix equation as

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{y} \tag{41}$$

we obtain the elements of $\mathbf{x}$ by inverting the matrix $\mathbf{A}$:

$$\mathbf{x} = \mathbf{A}^{-1} \cdot \mathbf{y}. \tag{42}$$

Once we have the estimated values for $\Delta P_{\rm c}$, $\Delta T_{\rm c}$, $\Delta R_{\rm s}$ and $\Delta L_{\rm s}$, we update the boundary conditions $P_{\rm c} \rightarrow P_{\rm c} - \Delta P_{\rm c}$, $T_{\rm c} \rightarrow T_{\rm c} - \Delta T_{\rm c}$, $R_{\rm s} \rightarrow R_{\rm s} - \Delta R_{\rm s}$, $L_{\rm s} \rightarrow L_{\rm s} - \Delta L_{\rm s}$ and compute the new solutions by integrating outwards and inwards to the midpoint. This procedure is repeated until convergence is achieved. Note the signs of the changes made to the boundary condition values above.

See the stellar structure code that is provided on the QMPlus page for this module to see how the above procedure is implemented in practice.