Numerical procedure

- Stellar differential equations, together with (realistic) material functions need to be solved numerically.
- There are two commonly used numerical procedures: the "shooting method" (including multiple shooting) and the "Henyey method".

Shooting method:

- one considers model in complete equilibrium at a given time and solves the "spatial problem" (4^{th}-order ODE system) for a given mass M and chemical profile $X_i(m)$.
- with 2 BCs at the centre (P_c, T_c) and 2 BCs at the surface (R, L) one integrates (shoots) from either boundaries (outwards and inwards) to match the 4 variables $r(m)$, $P(m)$, $T(m)$, $l(m)$ at a certain fitting point (e.g, base of convection zone) by varying all 4 BCs accordingly.
- nonlinearities (T^4, r^4,...) render numerical problem to be non-trivial.
- good for generating starting (guess) solution for relaxation methods.

Numerical procedure

Henyey method (Newton-Raphson-Kantorovich):

- This relaxation method is practical for solving boundary-value problems (BVP).
- A trial solution (e.g., obtained from the shooting method) is gradually improved in consecutive iterations (relaxations) until a predefined degree of accuracy is obtained (similarly to Newton's method).
- The PDEs are discretized by difference equ., & the corrections (Henyey matrix, Jacobians) are obtained from linearized algebraic equ.
- The spatial and time-dependent PDEs (+BCs and initial conditions at t_0) are solved as two subsystems separately and independently:

(1) 4 ODEs are solved for given $X_i(m)$ @ t,
(2) dX_i/dt is applied with a small time step Δt,
(3) followed by solving the 4 ODEs again for the new $X_i(m)$.

Numerical procedure

- in complete equilibrium ($\ddot{r} = P = T = 0$), the initial values are $X_i(m)$ and the PDEs simplify to 4 ODEs for the 4 unknown r, P, T, l in $[0,M]$.
- In hydrostatic equilibrium ($\ddot{r} = 0$) but thermal non-equilib. ($\dot{P} \neq 0, \dot{T} \neq 0$) the only difference (to above) is the additional term ε_g with the partial derivatives $\dot{P}$ and $\dot{T}$:→requires initial values @ t_0-Δt for $X_i(m)$, $P(m)$ and $T(m)$, e.g. $P^*(m), T^*(m)$, such that we can define derivatives:

$$\dot{P}_j = \frac{1}{\Delta t}(P_j - P_j^*), \quad \dot{T}_j = \frac{1}{\Delta t}(T_j - T_j^*)\,, \qquad \text{IV @ } t_0\text{-}\Delta t$$

at any point m=m_j in the stellar model.

For given Δt, P_j^*, T_j^* these time derivatives are now known and are functions of P_j and T_j only, similarly to material functions, e. g. $\varepsilon_g(P,T)$.
⟶ situation is now as before with complete equilibrium, i.e. 4 ODEs.

Numerical procedure

- Let's write these 4 ODEs as

$$\frac{dy_i}{dm} = f_i(y_1, \ldots, y_4), \quad i = 1, \ldots, 4\,,$$

where we have used the abbreviations $y_1 = r, y_2 = P, y_3 = T, y_4 = l$.

- Discretization: ODEs ⟶ difference equations for a finite mass interval $[m^j, m^{j+1}]$ denote the variables at both ends of this interval by upper indices, e.g.

$$y_1^j, y_1^{j+1}, \ldots, y_4^j, y_4^{j+1}.$$

The functions f_i on the right-hand sides to be taken for some average arguments (e.g. arithmetic or geometric mean of y_i^j and y_i^{j+1}):

$$f_i = f(y_i^{j+1/2})\,; \qquad f_i \simeq \frac{1}{2}[f(y_i^j) + f(y_i^{j+1})]$$

⟶ 4 ODEs become after conversion to difference equations:

$$A_i^j := \frac{y_i^j - y_i^{j+1}}{m^j - m^{j+1}} - f_i(y_1^{j+1/2}, \ldots, y_4^{j+1/2}), \quad i = 1, \ldots, 4\,,$$

Numerical procedure

4 ODEs become with:

$$A_i^j := \frac{y_i^j - y_i^{j+1}}{m^j - m^{j+1}} - f_i\left(y_1^{j+1/2}, \ldots, y_4^{j+1/2}\right), \quad i = 1, \ldots, 4\,,$$

the 4 difference equations (DE) in the mass interval m_j and m_{j+1}

$$A_i^j = 0, \quad i = 1, \ldots, 4\,.$$

These DEs represent a discretization of the ODEs and are therefore an approximation, the accuracy of which can be controlled by the value Δt and $\Delta m^j = m^j - m^{j-1}$.

not necessarily constant

Upper boundary @ m^1=m_F: $[P_F^{\rm in} = \pi(r_F^{\rm in}, L), \quad T_F^{\rm in} = \theta(r_F^{\rm in}, L)\,]$

with: $B_1 := y_2^1 - \pi\left(y_1^1, y_4^1\right), \quad B_2 := y_3^1 - \theta\left(y_1^1, y_4^1\right)\,,$

the upper BCs are

$$B_i = 0\,, \quad i = 1, 2\,.$$

Numerical procedure

j=K: **Central (inner-most) boundary**, i.e. interval between $m^K = 0$ and m^{K-1}:

from series expansion of all 4 variables about the centre:

$$r = \left(\frac{3}{4\pi\varrho_c}\right)^{1/3} m^{1/3}, \qquad l = (\varepsilon_n - \varepsilon_\nu + \varepsilon_g)_c\, m, \qquad P - P_c = -\frac{3G}{8\pi}\left(\frac{4\pi}{3}\varrho_c\right)^{4/3} m^{2/3}\,,$$

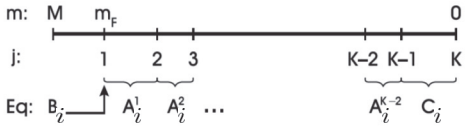
$$T^4 - T_c^4 = -\frac{1}{2ac}\left(\frac{3}{4\pi}\right)^{2/3} \kappa_c(\varepsilon_n - \varepsilon_\nu + \varepsilon_g)_c \varrho_c^{4/3} m^{2/3} \text{ (radiative)} + \text{(convective)}$$

$$\rightarrow \quad C_i\left(y_1^{K-1}, \ldots, y_4^{K-1}, y_2^K, y_3^K\right) = 0, \quad i = 1, \ldots 4\,,$$

which already include central values $y_1^K = y_4^K = 0$ (i.e. $r = l = 0$ at the centre).

Numerical procedure

Whole interval $m^K = 0, \ldots, m^1$: K-1 intervals on K meshpoints:



There are (4K-2) unknown variables ($y_1^K = y_4^K = 0$) with 2+4(K-2)+4 = 4K-2 equations:

outer BCs: $B_i(m^1)$ inner BCs: C_i

$$\begin{aligned} &B_i = 0, \quad i = 1, 2\,, \\ &A_i^j = 0, \quad i = 1, \ldots, 4, \quad j = 1, \ldots, K-2\,, \\ &C_i = 0, \quad i = 1, \ldots, 4\,. \end{aligned}$$

(note: this equations are nonlinear)

Numerical procedure

For given M, $X(m)$, $P^*(m)$, $T^*(m)$ and given trial (guess) solution $(y_i^j)_1$ with i=1,….,4, j=1,….,K we shall obtain

$$B_i(1) \neq 0, \quad A_i^j(1) \neq 0, \quad C_i(1) \neq 0\,,$$

where (1) indicates first iteration (approximation), because argument $(y_i^j)_1$ is only an approximation to the exact solution of the ODEs.

Corrections δy_i^j applied in the 2nd iteration (approximation)

$$\left(y_i^j\right)_2 = \left(y_i^j\right)_1 + \delta y_i^j$$

such that B_i, A_i^j and C_i vanish.

Corrections δy_i^j will bring about changes $\delta B_i, \delta A_i^j$, and δC_i, and we require

$$B_i(1) + \delta B_i = 0, \quad A_i^j(1) + \delta A_i^j = 0, \quad C_i(1) + \delta C_i = 0\,.$$

Numerical procedure

Corrections δy_i^j will bring about changes $\delta B_i, \delta A_i^j,$ and δC_i, and we require

$$B_i(1) + \delta B_i = 0, \quad A_i^j(1) + \delta A_i^j = 0, \quad C_i(1) + \delta C_i = 0 \, .$$

For **small enough** δy_i^j we can expand δB_i ,.... , to first order in δy_i^j , e.g.

$$\delta B_1 \approx \frac{\partial B_1}{\partial y_1^1}\delta y_1^1 + \frac{\partial B_1}{\partial y_2^1}\delta y_2^1 + \underbrace{\frac{\partial B_1}{\partial y_3^1}\delta y_3^1}_{\text{for } B_1 \text{ this is 0}} + \frac{\partial B_1}{\partial y_4^1}\delta y_4^1 \, .$$

(independent of y_3=*T*)

Numerical procedure

For small enough δy_i^j we can expand δB_i ,.... , to first order in δy_i^j , e.g.

$$\delta B_1 \approx \frac{\partial B_1}{\partial y_1^1}\delta y_1^1 + \frac{\partial B_1}{\partial y_2^1}\delta y_2^1 + \frac{\partial B_1}{\partial y_3^1}\delta y_3^1 + \frac{\partial B_1}{\partial y_4^1}\delta y_4^1 \, .$$

With this linearization the DE become a set of 4K-2 **linearized, inhomogeneous** equ.:

$$\frac{\partial B_i}{\partial y_1^1}\delta y_1^1 + \cdots + \frac{\partial B_i}{\partial y_4^1}\delta y_4^1 = -B_i, \qquad i = 1, 2 \, ,$$

$$\frac{\partial A_i^j}{\partial y_1^j}\delta y_1^j + \cdots + \frac{\partial A_i^j}{\partial y_4^j}\delta y_4^j + \frac{\partial A_i^j}{\partial y_1^{j+1}}\delta y_1^{j+1} + \cdots + \frac{\partial A_i^j}{\partial y_4^{j+1}}\delta y_4^{j+1} = -A_i^j, \qquad \begin{matrix} i = 1, \ldots, 4, \\ j = 1, \ldots, K-2 \, , \end{matrix}$$

$$\frac{\partial C_i}{\partial y_1^{K-1}}\delta y_1^{K-1} + \cdots + \frac{\partial C_i}{\partial y_4^{K-1}}\delta y_4^{K-1} + \frac{\partial C_i}{\partial y_2^K}\delta y_2^K + \frac{\partial C_i}{\partial y_3^K}\delta y_3^K = -C_i \, , \qquad i = 1, \ldots, 4 \, .$$

for the 4K-2 unknown corrections δy_i^j ($\delta y_1^K = \delta y_4^K = 0$) .

In matrix form we write:

$$H \begin{pmatrix} \delta y_1^1 \\ . \\ . \\ . \\ \delta y_3^K \end{pmatrix} = - \begin{pmatrix} B_1 \\ . \\ . \\ . \\ C_4 \end{pmatrix} .$$

Henyey matrix (= partial derivatives [Jacobians])

Numerical procedure

In matrix form we write

$$H \begin{pmatrix} \delta y_1^1 \\ . \\ . \\ . \\ \delta y_3^K \end{pmatrix} = - \begin{pmatrix} B_1 \\ . \\ . \\ . \\ C_4 \end{pmatrix} .$$

det(*H*) is typically non-singular (det(*H*) ≠ 0), so that this linear system can be solved for the wanted corrections δy_i^j, to obtain a more accurate solution in the next iteration (relaxation) step

$$(y_i^j)_2 = (y_i^j)_1 + \delta y_i^j \, .$$

Even after the 2nd iteration we still get

$$B_i(2) \neq 0, \quad A_i^j(2) \neq 0, \quad C_i(2) \neq 0 \, ,$$

because the corrections were linearized and the full set of equations are nonlinear.

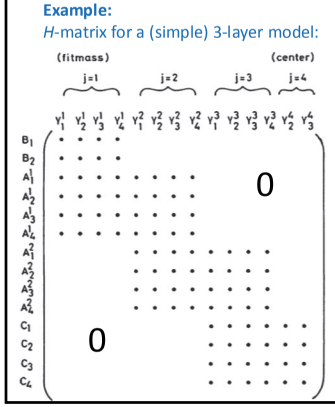
$\longrightarrow$ $(y_i^j)_3 = (y_i^j)_2 + \delta y_i^j$, and so on, until e.g., $\Sigma|\delta y_i^j| < \epsilon \simeq 10^{-12}$.

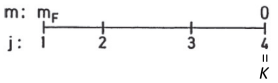
Numerical procedure

- For a (time-)evolutionary model one updates now the $X_i(2)=X_i(1)+\Delta t\, \dot{X}_i(1)$ (i.e. an explicit scheme) and [*P*(*m*), *T*(*m*)] ⟶ [*P**(*m*), *T**(*m*)] for the new $t+\Delta t$, and the new spatial model at $t+\Delta t$ is obtained, as for the previous time *t*, from the Henyey method.

Example:

H-matrix for a (simple) 3-layer model:





Diagonal *(4K-2)* x (*4K-2)* matrix needs to be inverted.

The Henyey method needs *K* inversions of matrices of size 4x8 (*J*x2*J*; 2x4, 4x6).

ODE-order

There are also other algorithms available (e.g., Gauss-Seidel, etc.).

- ≙ e.g., $\partial A_k^l / \partial y_i^j$

Numerical procedure: $\partial/\partial t$, $\partial^2/\partial t^2$

1st-order derivatives $\partial/\partial t$:

- explicit scheme: time interval $t^n \rightarrow t^{n+1}$

@ t^{n+1}: $X_i^{n+1} = X_i^n + \Delta t \dot{X}_i^n$,

with $\dot{X}_i^n = \frac{m_i}{\rho^n}\left(\Sigma_j r_{ji}^n - \Sigma_j r_{ik}^n\right)$.

note: in an explicit scheme $\Delta t \leq \Delta r / v_s$ (Courant condition), where v_s is the (local) speed of sound.

- implicit scheme: time interval $t^n \rightarrow t^{n+1}$

@ t^{n+1}: $X_i^{n+1} = X_i^n + \Delta t \dot{X}_i^{n+1}$,

with $\dot{X}_i^{n+1} = \frac{m_i}{\rho^{n+1}}\left(\Sigma_j r_{ji}^{n+1} - \Sigma_j r_{ik}^{n+1}\right) = \dot{X}_i(X_j^{n+1})$,

note (nonlinear): $\rho(X_k)$, $r_{ji}(X_k)$,

and p^{th} - iterated solution @ t^{n+1} (e.g., fixed-point iteration):

$$X_i^{n+1}(0) = X_i^n \quad ; X_i^{n+1}(p+1) = X_i^n + \Delta t \dot{X}_i(X_j^{n+1}(p)) ,$$

or using a Henyey-like (Newton-Raphson-Kantorovich) method to obtain $X_i^{n+1}(p+1)$.

Numerical procedure: $\partial/\partial t$, $\partial^2/\partial t^2$

- implicit scheme: time interval $t^n \rightarrow t^{n+1}$

Note: in energy equation (ε_g) we also had an implicit time-derivative:

$$\dot{P} = \frac{P^{n+1} - P^n}{\Delta t} , \qquad \dot{T} = \frac{T^{n+1} - T^n}{\Delta t} .$$

2nd-order derivatives $\partial^2/\partial t^2$:

In momentum equation we have for the so-called hydrodynamical problem:

$$\frac{\partial P}{\partial m} = -\frac{Gm}{4\pi r^4} - \frac{1}{4\pi r^2}\frac{\partial^2 r}{\partial t^2} .$$

By introducing a **new variable** (velocity) and new differential equation

$$v = \frac{\partial r}{\partial t}$$

we obtain

$$\frac{\partial P}{\partial m} = -\frac{Gm}{4\pi r^4} - \frac{1}{4\pi r^2}\frac{\partial v}{\partial t} ,$$

i.e., we transformed one 2nd-order differential eq. into two 1st-order differential equations.

Numerical procedure: diffusion equation

$$\frac{\partial X_i}{\partial t} = -\frac{1}{\rho r^2}\frac{\partial}{\partial r}\left[r^2 X_i T^{5/2}\left(A_P(i)\frac{\partial \ln p}{\partial r} + A_T(i)\frac{\partial \ln T}{\partial r} + \sum_{k \neq e, \mathrm{He}^4} A_k(i)\frac{\partial \ln C_i}{\partial r}\right)\right] .$$

- includes 1st – order time derivative and 2nd – order spatial derivatives.

- 1st – order time derivative can be solved similarly as for the nuclear network eq., i.e. the system of equations for the *N* (diffusive) species can be solved with either an explicit or implicit method.

- 2nd – order spatial derivatives, e.g. ln *T*, can be solved in two steps:

@ grid point *j* $\frac{\Delta \ln T^j}{\Delta r^j} = \frac{\ln T^j - \ln T^{j-1}}{r^j - r^{j-1}}$ and similarly @ *j*+1 .

from which the 2nd – order derivative @ *j* is calculated from

$$\left.\frac{\partial^2 \ln T}{\partial r^2}\right|_j \approx \left(\frac{\Delta \ln T^{j+1}}{\Delta r^{j+1}} - \frac{\Delta \ln T^j}{\Delta r^j}\right) / \left(\bar{r}^{j+1} - \bar{r}^j\right) ,$$

where $\bar{r}^j$ is a suitable mean value for r in the interval $(j, j+1)$. In the simplest case it is the arithmetic mean and thus the denominator reduces to $(r^{j+1} - r^{j-1})/2$.

Numerical procedure: diffusion equation

$$\frac{\partial X_i}{\partial t} = -\frac{1}{\rho r^2}\frac{\partial}{\partial r}\left[r^2 X_i T^{5/2}\left(A_P(i)\frac{\partial \ln p}{\partial r} + A_T(i)\frac{\partial \ln T}{\partial r} + \sum_{k \neq e, \mathrm{He}^4} A_k(i)\frac{\partial \ln C_i}{\partial r}\right)\right] .$$

from which the 2nd – order derivative @ *j* is calculated from

$$\left.\frac{\partial^2 \ln T}{\partial r^2}\right|_j \approx \left(\frac{\Delta \ln T^{j+1}}{\Delta r^{j+1}} - \frac{\Delta \ln T^j}{\Delta r^j}\right) / \left(\bar{r}^{j+1} - \bar{r}^j\right) ,$$

where $\bar{r}^j$ is a suitable mean value for r in the interval $(j, j+1)$. In the simplest case it is the arithmetic mean and thus the denominator reduces to $(r^{j+1} - r^{j-1})/2$.

All other quantities to be differentiated only once, e.g. A_P, A_T, A_k, have also to be taken as mean quantities for the 2nd – derivative in analogy to the 2nd – order derivative of *T* shown above.

Note that these spatial derivatives are defined here at each grid point *j*, where as the derivatives (r.h.s.) of the discretized stellar structure equations were defined between *j* and *j*+1, which we indicated as "*j*+1/2". The diffusion equations are defined at the same grid locations as the nuclear network.

Numerical procedure: diffusion equation

$$\frac{\partial X_i}{\partial t} = -\frac{1}{\rho r^2}\frac{\partial}{\partial r}\left[r^2 X_i T^{5/2}\left(A_P(i)\frac{\partial \ln p}{\partial r} + A_T(i)\frac{\partial \ln T}{\partial r} + \sum_{k\neq e,\mathrm{He}^4} A_k(i)\frac{\partial \ln C_i}{\partial r}\right)\right].$$

The so discretized *N* diffusion equations for *N* species at the *j*=2,...,*K*-1, i.e. *K*-2 grid points are solved by a Newton-Raphson-Kantorovich iteration for $X_i(t+\Delta t)$, starting from an initial trial value $X_i(t)$. The now **3 connected**, **neighbouring grid points** (from the 2nd - order spatial derivatives) increase the block matrices in the Henyey method to *N* x **3***N*.

Remaining two equations to complete system for the *N* species from BCs at *j*=1 and *j*=*K*. From the conservation equ. (Schlattl 1999) we get

element (species)

grid point

$$\sum_{j=1}^{K}\left(X_i^j(t+\Delta t) - X_i^j(t)\right)\triangle m^j = 0, \qquad 1 \le i \le N$$

leading to BCs as shown here only for ln *T* (Schlattl 1999) ($K_T := r^2 X_i(t+\Delta t) T^{5/2} A_T$)

$$\frac{1}{\varrho r^2}\frac{\partial}{\partial r}\left(K_T\frac{\partial \ln T}{\partial r}\right)_{r=R} \approx -\frac{2}{\varrho^{j=1}R^2}\frac{\bar{K}_T^{j=2}(\Delta \ln T/\Delta r)^{j=2}}{r^{j=1} - r^{j=2}}$$

and

$$\frac{1}{\varrho r^2}\frac{\partial}{\partial r}\left(K_T\frac{\partial \ln T}{\partial r}\right)_{r=0} \approx \frac{24}{\varrho^{j=K}(r^{j=K-1})^2}\frac{\bar{K}_T^{j=K}(\Delta \ln T/\Delta r)^{j=K}}{r^{j=K-1}}.$$

Numerical procedure: mass loss

Mass loss formula (e.g., Reimers 1975):

$$\dot{M}_{\mathrm{R}} = -4\cdot 10^{-13}\eta\frac{L}{gR}\cdot\frac{g_\odot R_\odot}{L_\odot}$$

- over time step Δt, during which $X_i(m)$ changes, the stellar mass changes as

$$M(t+\Delta t) = M(t) - \Delta M(t) = M(t) - \dot{M}(t)\Delta t,$$

where $\dot{M}(t)$ is the mass loss rate calculated according to Reimer's (or other's) expression, and using the stellar parameters at time *t*.

- grid points i with mass $m_i \geq M(t) - \Delta M(t)$ are simply "removed", which ignores dynamical effects such as accelerating matter and necessary energy $(\dot{M}GM)/R$ erg/s to remove mass from the gravitational potential *GM*/*R* (Sun: 10^{-7} $L_\odot$, but in evolved red giants: 1% of *L*).

- changes in thermal structure, as a result of removing grid points, is also typically ignored, which is ok as long as $\dot{M}/M \gg \tau_{\mathrm{KH}}$ ($(\dot{M}/M)_\odot \simeq 10^{14}$).