

Domain of applicability: Pre Main Sequence to Post Main Sequence

1. Basic structure of code

1. Mesh in mass $M(i), i = 0, N$; structure variables $V_j(i)$, Chemical Species $X_k(i)$
2. At time t , predict values V_j, X_j at $t + dt$, calculate new X_k at $t + dt$
3. Solve structure for V_j at $t + dt$ with new X_j
4. Iterate steps 2 and 3 to convergence.

$$V_j = r, L, \rho, T, P, U, \dots; :X_k(k = 1, 9) = {}^1H, {}^3He, {}^4He, {}^{12}C, {}^{13}C, {}^{14}N, {}^{15}N, {}^{16}O, {}^{17}O$$

2. Structure equations in form solved in code

$$\frac{\partial M_r}{\partial r^3} = \frac{4}{3}\pi G\rho, \quad \frac{\partial L_r}{\partial M_r} = \epsilon - \left[\frac{\partial U}{\partial t} - \frac{P}{\rho^2} \frac{\partial \rho}{\partial t} \right], \quad \frac{\partial T}{\partial r^2} = -\nabla \frac{T}{P} \frac{GM_r \rho}{2r^3}$$

$$\nabla \equiv \frac{\partial \log T}{\partial \log P} = \nabla_{rad} \text{ (if } \leq \nabla_{ad} \text{) else } = \nabla_{con}. \quad \nabla_{rad} = \frac{3L_r P \kappa}{64\pi \sigma G M_r T^4}, \quad \nabla_{con} \text{ from } MLT$$

MLT Convective Model as implemented in this code, $\ell = \alpha H_p$

$$\nabla_{con} = \nabla_{ad} + \Delta \nabla, \quad \Delta \nabla = \left(\frac{2\rho B^2}{\lambda P} \right) (x^2 + x), \quad B = \frac{48\sigma T^3}{c_p \kappa \alpha^2 H \rho^2}, \quad \lambda = - \left(\frac{\partial \log \rho}{\partial \log T} \right)_P$$

$$x^3 + \frac{4}{9} (x^2 + x) = \frac{2}{9} \left(\frac{\lambda P}{\rho B^2} \right) (\nabla_{rad} - \nabla_{ad}), \quad H = \min \left(\frac{P}{\rho h \sigma g}, \left(\frac{rP}{2\rho g} \right)^{1/2} \right), \quad v_{con} = \frac{1}{2} \alpha B x$$

3. Equation state and opacity

OPAL GN93 + Alexander opacities, OPAL 2001 state tables, converted for given Z to tables for $\log P, \log U, \log Cp, \lambda, \nabla_{ad}, \Gamma_1, \log \kappa$ vs $[\log T, \log(\rho/T^3)]$. Interpolation by local cubics with continuous 1st derivatives. Minor species composition as in tables.

4. Surface layers - Atmosphere

Eddington grey atmosphere incorporated in model by imposing surface condition at $R = r(N)$ where optical depth $\tau = \tau_s \sim 0.001$

$$T^4(N) = \frac{L(N)}{4\pi \sigma R^2} \left(\tau_s + \frac{2}{3} \right), \quad P(N) = \frac{GM(N)}{R^2} \frac{\tau_s}{\kappa(N)}$$

Photosphere determined by iterative interpolation to find the value of R_{ph} where $T = T_{eff}$ with $T_{eff}^4 = L(N)/(4\pi \sigma R_{ph}^2)$.

5. Convective Core

Nearest mesh points relocated to core boundary ($\nabla_{rad} = \nabla_{ad}$) and to overshoot boundary during successive iterations for structure and chemical evolution.

Chemical profiles outside *shrinking* cores smoothed linearly in M_r from $M_c(t)$ to $M_c(t+dt)$

Chemical overshooting only, extends mixed region by $\beta \min(H, r_c)$.

6. Condensed Nuclear reaction network used in this code

$R_{ij}X_iX_j$ = number of reactions/gm/sec of species i with species j Reaction rates R_{ij} and energy release Q_{ij} from NACRE with ν, β decay from Bahcall. New analytic fit to weak-intermediate-strong screening.

$$R_{11} : {}^1H(p, \nu e^+) {}^2H(p, \gamma) {}^3He$$

$$R_{33} : {}^3He({}^3He, \alpha 2p) {}^4He$$

$$R_{43} : {}^3He(\alpha, \gamma) {}^7Be(e^-, \nu) {}^7Li(p, \alpha) {}^4He$$

$$R_{121} : {}^{12}C(p, \gamma) {}^{13}N(, e^+ \nu) {}^{13}C$$

$$R_{131} : {}^{13}C(p, \gamma) {}^{14}N$$

$$R_{141} : {}^{14}N(p, \gamma) {}^{15}O(, e^+ \nu) {}^{15}N$$

$$R_{151} : {}^{15}N(p, \gamma \alpha) {}^{12}C$$

$$R_{151a} : {}^{15}N(p, \gamma) {}^{16}O$$

$$R_{161} : {}^{16}O(p, \gamma) {}^{17}F(, e^+ \nu) {}^{17}O$$

$$R_{171} : {}^{17}O(p, \gamma \alpha) {}^{14}N$$

7. Chemical evolution equations

Mixing in convective regions is modelled as a diffusion process with the diffusion coefficient ν_c determined by the MLT model of convection $\nu_c = v_{con}\ell/3$

$$\frac{\partial X_k}{\partial t} = m_i \sum N_{ijk} R_{ij} X_i X_j + \frac{1}{\rho r^2} \frac{\partial}{\partial r} \left(\rho \nu_c r^2 \frac{\partial X_k}{\partial r} \right)$$

where N_{ijk} is the number of particles of species k produced in reaction R_{ij}

Solving the chemical evolution equations for X_k

At mesh point i the diffusion term is discretised in conservative form as

$$-\frac{dt}{\rho r^2} \frac{\partial}{\partial r} \left(\rho \nu_c r^2 \frac{\partial X_k}{\partial r} \right)_i = A_p[X_k(i+1) - X_k(i)] - A_m[X_k(i) - X_k(i-1)]$$

The evolution equations form a set of tridiagonal equations for each k of the form

$$A_p(i)X_k(i+1) + A_{0k}(i)X_k(i) + A_m(i)X_k(i-1) = S_k(i), \quad i = 0, N; \quad k = 1, 9$$

where A_{0k} and S_k depend on the values of V_j, X_j at time $t + dt$ and V_{0j}, X_{0j} at time t , The equations are solved using a 1st order implicit algorithm (of which there are many varieties!).

The equations are solved sequentially; that is for each k we solve the system for $i = 0, N$ using a tridiagonal matrix solver, and the set whole set is repeatedly solved with the updated $X_j(i)$ until the solution for the $X_k(i)$ has converged here defined as

$$\sum_i [\delta X_1(i)]^2 + 10^6 \sum_i [\delta X_3(i)]^2 + 10^4 \sum_{k \neq 1, 3} \sum_i [\delta X_k(i)]^2 < acc \quad (\sim 10^{-10})$$

where δX_k is the difference in values of X_k between successive iterations.

8. Solving structure equations give X_k

The variables $V_1(i) = r, V_2(i) = L_r, V_3(i) = \rho, V_4(i) = T$; all other state variables are known in terms of these variables and the values of $X_k(i)$ and Z

The time derivatives $\partial Q/\partial t$ are taken as 1^{st} order implicit in time, and the differential equations are discretised to 2^{nd} order in space in the form:

$$E_1(i) = [M_{i+1} - M_i] - \frac{1}{2} \left[\left(\frac{dM_r}{dr^3} \right)_i + \left(\frac{dM_r}{dr^3} \right)_{i+1} \right] [r_{i+1}^3 - r_i^3]$$

$$E_2(i) = [L_{i+1} - L_i] - \frac{1}{2} \left[\left(\frac{dL_r}{dM_r} \right)_i + \left(\frac{dL_r}{dM_r} \right)_{i+1} \right] [M_{i+1} - M_i]$$

$$E_3(i) = [T_{i+1} - T_i] - \frac{1}{2} \left[\left(\frac{dT}{dr^2} \right)_i + \left(\frac{dT}{dr^2} \right)_{i+1} \right] [r_{i+1}^2 - r_i^2]$$

$$E_4(i) = \log \left(\frac{T_{i+1}}{T_i} \right) - \frac{1}{2} [\nabla_{i+1} - \nabla_i] \log \left(\frac{P_{i+1}}{P_i} \right)$$

The equations are satisfied when $E_k(i) = 0, k = 1, 4; i = 1, N-1$ plus the central boundary conditions ($r = 0, L_r = 0$ at $M_r = 0$, and the surface boundary conditions given by the atmosphere (section 4 above).

The $E_k(i)$ depend on the variables at $V_j(i), V_j(i+1), j = 1, 4$. We iterate to find the values of the V_j that give $E_k(i) = 0$ using a Newton-Raphson technique.

At any given iteration $E_k(i) \neq 0$. We find the derivatives of the $E_k(i)$ wrt $V_j(i), V_j(i+1)$, and solve the linearised equations for corrections $\delta V_j(i)$

$$\frac{\partial E_k(i)}{\partial V_j(i)} \delta V_j(i) + \frac{\partial E_k(i)}{\partial V_j(i+1)} \delta V_j(i+1) = -E_k(i)$$

which can be written as

$$A_{kj}(i) \delta V_j(i) = -E_k(i)$$

where A is a block diagonal matrix, the blocks being 8×4 . This system is readily solved by elimination of the first 2 columns in each block, diagonalisation of the 4×4 square section of the block, and back substitution. This gives corrections $\delta V_j(i)$ to be added to the $V_j(i)$ This process is repeated until the solution has converged.

In practice we use $\log V$ rather than V and the solution is deemed to be converged when all corrections $\delta V/V < acc$ ($\sim 1/N^2$).

Results

The results for the ESTA comparison models are given in the poster by Montiero et al. Here we point out that relocating a mesh point at the boundary of convective cores and of any overshoot region results in a relatively smooth variation of the Brunt-Väisälä frequency. This is illustrated in the figure which shows the results of applying this code to Case 1.5 of the ESTA comparison exercise. This is for a star of $M = 2.0M_\odot, X_0 = 0.72, Z = 0.02$ with an overshoot parameter $\beta = 0.15$ evolved to a central hydrogen abundance of $X_c = 0.01$.

Figure 1 $M=2.0M_{\odot}$, $X_0=0.720$, $Z=0.020$, $t=1.198E+09y$ Fixed mesh points

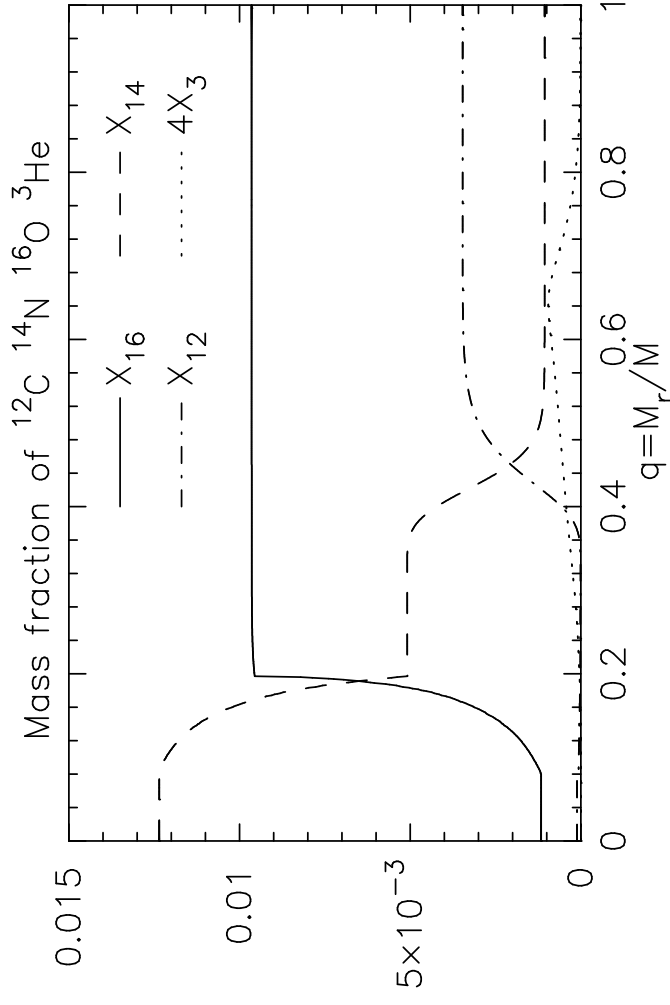
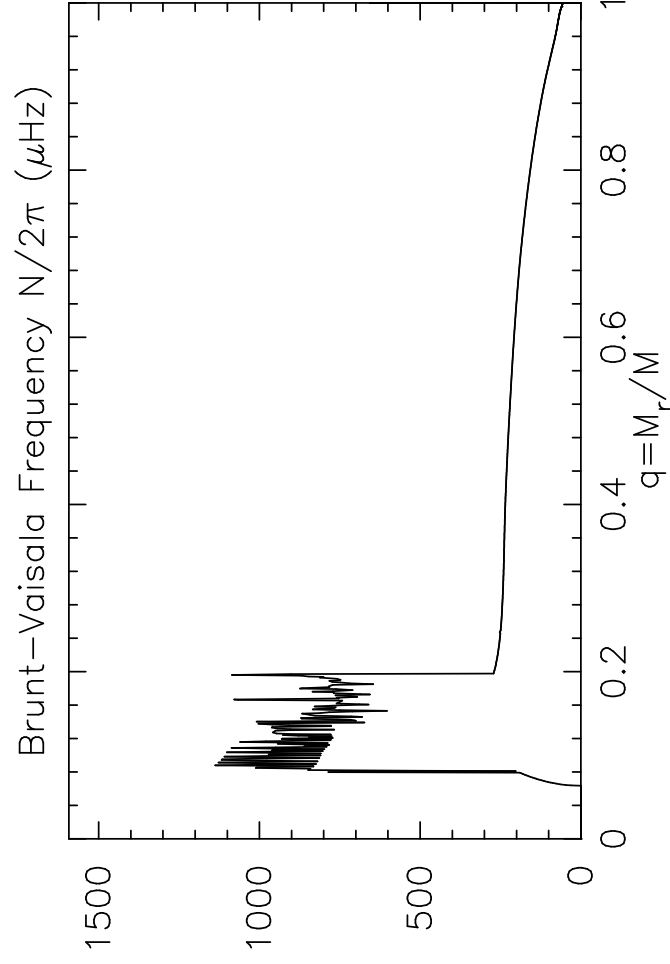
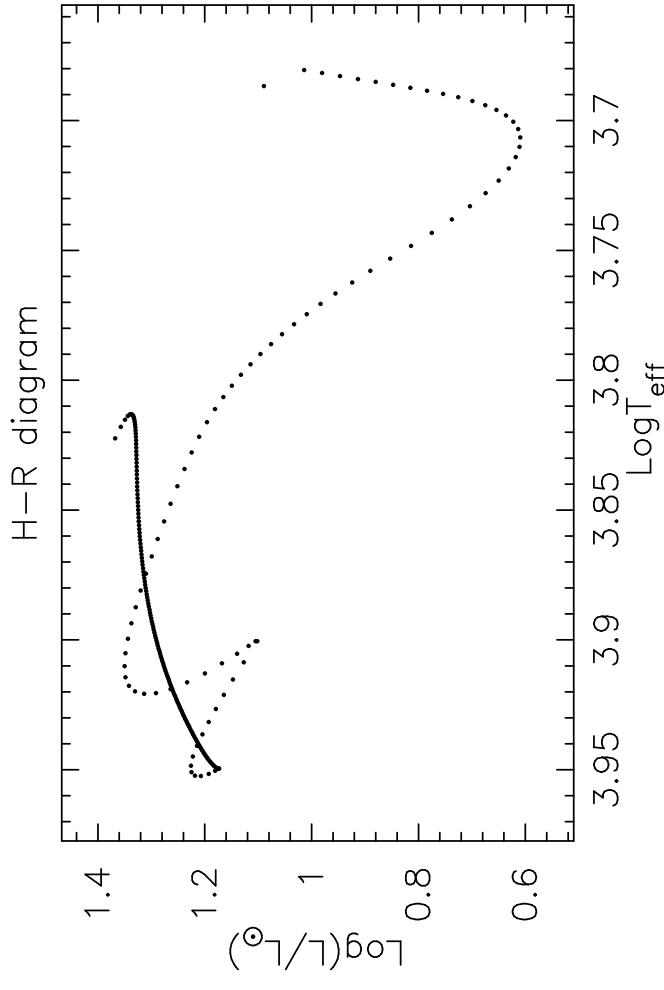
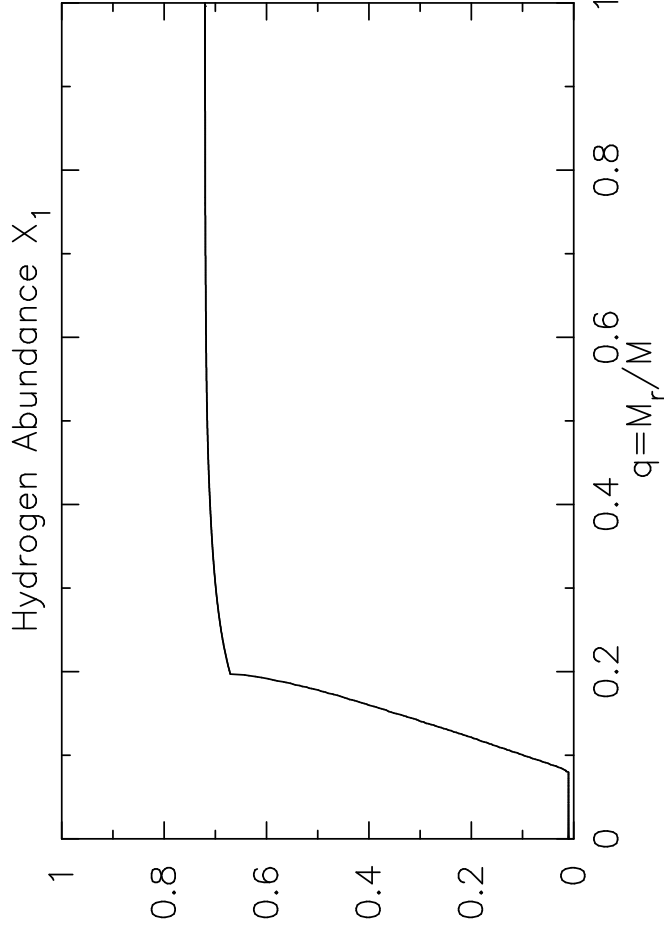


Figure 2 $M=2.0M_{\odot}$, $X_0=0.720$, $Z=0.020$, $t=1.200E+09y$ Relocated boundary point

