starox-NACRE17: stellar evolution code

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Domain of applicability: Pre Main Sequence to Post Main Sequence

Basic structure of code

1. Mesh in mass $M(i), i = 0, N; dM(i) = M(i) - M(i-1)$
2. At time t, $V_0(j,i)$ are the structure variables j at mesh point i
   $X_0(k,i)$ the composition variables k at i
3. Guess $V(j,i), X(k,i)$ at $t + dt$ [here taken as $V_0(j,i), X_0(k,i)$]
4. Solve chemistry for $X(k,i)$ at $t + dt$ using $V(j,i), V_0(j,i), X(k,i), X_0(k,i)$
5. Solve structure for $V(j,i)$ at $t + dt$ given $X(j,i), V_0(j,i)$

   Iterate steps 4 and 5 to find $V(j,i), X(j,i)$ at $t + dt$

Structure Variables: $V1 = r,\ V2 = L,\ V3 = \rho,\ V4 = T,\ V5 = P,\ V6 = U, \ldots$
Chemical species: $^1H,\ ^3He,\ ^4He,\ ^{12}C,\ ^{13}C,\ ^{14}N,\ ^{15}N,\ ^{16}O,\ ^{17}O,\ Z$

Structure equations in form solved in code

$$\frac{\partial M_r}{\partial r^3} = \frac{4}{3}\pi G\rho$$

$$\frac{\partial L_r}{\partial M_r} = \epsilon - \left[\frac{\partial U}{\partial t} - \frac{P}{\rho^2}\frac{\partial \rho}{\partial t}\right]$$

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

$$= \nabla_{con} \text{ if } \nabla_{rad} > \nabla_{ad}, \quad \nabla_{con} \text{ from MLT}$$

$$\frac{\partial T}{\partial r^2} = \nabla \frac{T}{P}\frac{\partial P}{\partial r^2} = -\nabla \frac{T}{P}\frac{G M_r \rho}{2r^3}$$

$P = P(\rho, T, X_1, Z),\ U = U(\rho, T, X_1, Z),\ \nabla_{ad} = \nabla_{ad}(\rho, T, X_1, Z)$

$\kappa = \kappa(\rho, T, X_1, Z),\ \epsilon = \epsilon(\rho, T, X_k, Z)$

Other forms of equations readily implemented

MLT Convective Model as implemented in this code

α is mixing length parameter $\ell = \alpha H$

$$\nabla_{con} = \nabla_{ad} + \Delta\nabla, \quad \Delta\nabla = \left(\frac{2\,\rho B^2}{\lambda P}\right)\left(x^2 + x\right)$$

$$B = \frac{48\sigma T^3}{c_p \kappa \alpha^2 H \rho^2}, \quad \lambda = -\left(\frac{\partial \log \rho}{\partial \log T}\right)_P$$

$$x^3 + \frac{4}{9}\left(x^2 + x\right) = \frac{4}{9}\left(\frac{\lambda\, P}{2\,\rho B^2}\right)\left(\nabla_{rad} - \nabla_{ad}\right) = W$$

$$H = min(H_p, H_2), \quad H_p = \frac{-P}{dP/dr}, \quad H_2 = \sqrt{\frac{-P}{dP/dr^2}}$$

$$v_{con} = \frac{1}{2}\,\alpha\,B\,x \quad \ell = \alpha\,H, \quad \nu_c = \frac{1}{2}\,\ell\,v_{con}$$

$$\text{Solution for } x: \quad x_1 = \frac{9W}{(8+27W)^{2/3}}, \quad x_{k+1} = \left(\frac{W + 2x_k^3 + 4x_k^2/9}{3x_k^2 + 8x_k/9 + 4/9}\right), k = 3$$

Energy generation

$\epsilon = \sum R_{jk} X_k X_j E_{kj}$ Rates R_{kj}, energy/reaction E_{kj}

$R_{kj} X_k X_j$=Number of Reactions/gm/sec of species k with j

Here R_{kj}, E_{kj} from NACRE (usually Adelberger); ν, β decay Bahcall.

Includes iwr fit to weak-intermediate-strong screening.

Equation state and opacity

OPAL GN93 + Alexander opacities, OPAL 2001 state tables.

Generate Ztables on uniform mesh in $VLT = \log_{10} T,\ VLR = \log_{10}(\rho/T^3),\ X_1$

$VLT = 3.30\ (0.05)\ 8.5 \quad VLR = -25.0\ (0.125)\ -17.0 \quad X_1 = 0\ (0.1)\ 1.0$

Data tabulated:

$VLP = \log_{10} P,\ \ VLU = \log_{10} U,\ \ VLCp = \log_{10} Cp$

$$VLRT = \left(\frac{\partial \log \rho}{\partial \log T}\right)_P, \quad \nabla_{ad}, \quad \Gamma_1, \quad VLK = \log_{10} \kappa$$

Interpolation is by local 4 point cubics with continuous 1st derivatives.

Composition: fixed as in state and opacity tables.

Chemical Evolution

Condensed Nuclear reaction network used in this code

R_{kj} : Number of Reactions/gm/sec of species k with $j = R_{kj} X_k X_j$
E_{kj} : Net energy (ergs) released to gas per reaction of species k with j
includes e^+ anihilation, less ν losses.

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

Evolution equations

Mixing in convective regions is modelled as a diffusion process with the diffusion coefficient $\nu_c =$ determined by the MLT model of convection.

$$\frac{\partial X_1}{\partial t} = \big[2R_{33}X_3^2 - 3R_{11}X_1^2 - R_{43}X_4X_3 - X_1\ \big(R_{121}X_{12} + R_{131}X_{13} + R_{141}X_{14}$$
$$+R_{151}X_{15} + R_{151a}X_{15} + R_{161}X_{16} + R_{171}X_{17}\big)\big]m_H + \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left(\rho\nu_c r^2 \frac{\partial X_1}{\partial r}\right)$$

$$\frac{\partial X_3}{\partial t} = \big[R_{11}X_1^2 - 2R_{33}X_3^2 - R_{43}X_4X_3\big]m_3 + \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left(\rho\nu_c r^2 \frac{\partial X_3}{\partial r}\right)$$

$$\frac{\partial X_4}{\partial t} = \big[R_{33}X_3^2 + R_{43}X_4X_3 + R_{151}X_{15}X_1\big]m_4 + \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left(\rho\nu_c r^2 \frac{\partial X_4}{\partial r}\right)$$

$$\frac{\partial X_{12}}{\partial t} = \big[R_{151}X_{15}X_1 - R_{121}X_{12}X_1\big]m_{12} + \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left(\rho\nu_c r^2 \frac{\partial X_{12}}{\partial r}\right)$$

$$\frac{\partial X_{13}}{\partial t} = \big[R_{121}X_{12}X_1 - R_{131}X_{13}X_1\big]m_{13} + \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left(\rho\nu_c r^2 \frac{\partial X_{13}}{\partial r}\right)$$

$$\frac{\partial X_{14}}{\partial t} = \big[R_{131}X_{13}X_1 + R_{171}X_{17}X_1 - R_{141}X_{14}X_1\big]m_{14} + \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left(\rho\nu_c r^2 \frac{\partial X_{14}}{\partial r}\right)$$

$$\frac{\partial X_{15}}{\partial t} = \big[R_{141}X_{14}X_1 - R_{151}X_{15}X_1 - R_{151a}X_{15}X_1\big]m_{15} + \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left(\rho\nu_c r^2 \frac{\partial X_{15}}{\partial r}\right)$$

$$\frac{\partial X_{16}}{\partial t} = \big[R_{151a}X_{15}X_1 - R_{161}X_{16}X_1\big]m_{16} + \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left(\rho\nu_c r^2 \frac{\partial X_{16}}{\partial r}\right)$$

$$\frac{\partial X_{17}}{\partial t} = \big[R_{161}X_{16}X_1 - R_{171}X_{17}X_1\big]m_{17} + \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left(\rho\nu_c r^2 \frac{\partial X_{17}}{\partial r}\right)$$

Surface layers - Atmosphere

No separate atmosphere

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

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

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

Slight error due to height of atmosphere ($\tau \neq \tau_s$)

Interpolate for values of all variables V_j, X_k at R_{ph} and intercalate in the output model.

Convective Core

Boundary of core $M_r = M_c,\ r = r_c$

Relocate nearest mesh point to core boundary

During iterations for structure determine boundary of core M_c where $\nabla_{rad} = \nabla_{ad}$ by interpolation

Move nearest mesh point to core boundary, interpolate values of variables M, dM, V, V_0, X, X_0 on core boundary.

Include $|M_c(it)/M_c(it-1)| < acc$ in convergence condition for structure

Smoothing chemical profile outside shrinking core

Chemical profiles outside *shrinking* core linear in M_r from $M_c(t)$ to $M_c(t+dt)$

Overshooting from convective core, chemical mixing only

Extends mixed region by $\beta\, min(H, r_c)$ setting ν_c constant in overshoot region from r_c to r_{ov}. β adjustable parameter.

Advancing the solution from t to $t + dt$

The basic solution algorithm is implemented as follows

```
1     call predict(M,V,Vo,X,Xo,t,dt,N,Nv,Nm)
      do k=1,kk
            call newxi(M,dM,V,Vo,X,Xo,dt,Z,N,Nv,Nm,kt)
            call Xmodel(M,dM,V,Vo,X,Xo,dt,Z,N,Nv,Nm,it)
            if(it.eq.1) goto 4
      enddo
4     continue
      if(X(1,0).gt.Xend) goto 1
```

subroutine predict sets the time step dt, stores values at t in $X_0(k,i), V_0(j,i)$, predicts $X(k,i), V(j,i)$ at $t+dt$ [here set equal to $X_0(k,i), V_0(j,i)$].

subroutine newxi calculates new values of $X(k,i)$ using the input values of V, V_0, X, X_0. kt is the number of iterations needed in **newxi** for the solution for the new $X(k,i)$ to converge.

subroutine Xmodel then calculates new values of $V(j,i)$ using the input values of V, V_0, X. it is the number of iterations needed in **Xmodel** for the solution for the new $V(j,i)$ to converge.

The cycle is repeated until the solution for the $V(j,i)$ has converged ($it = 1$).

Solving the Chemical equations for $X(k, i)$

The chemical evolution equations are solved as 1st order implicit equations;

$$\left(\frac{\partial X_k}{\partial t}\right)_i = \frac{X_k(i) - X_{ko}(i)}{dt}$$

the diffusion term being expressed in conservative form as

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

$A_p(i), A_m(i)$, which are the same for all k can be very large in convective regions; in practice they are limited in magnitude for reasons of numerical accuracy. The evolution equations are then written as a set of linear tridagonal equations for each k of the form

$$A_p(i)X_k(i+1) + A_0(i)X_k(i) + A_m(i)X_k(i-1) = S_k(i), \quad i = 0, N$$

where $A_0(i)$ and $S_k(i)$ depend on the values of the of $A_m(i), A_p(i), R_{ij}, V(j,i)$, $X(j,i), X_0(j,i)$ whose current values are known on entry to **newxi**.

An example is the equation for X_3 which is here updated using the code

```
      call rates(V,R11,R33,...
      call difcof(M,dM,V,AP,AM,..

*     advance X3
      do i=0,N
         A0(i)=1-AP(i)-AM(i)+(R33(i)*(X3(i)+X3o(i))+R43(i)*X4(i))*m3*dt
         S(i)=X3o(i)+R11(i)*X1(i)*X1o(i)*m3*dt
      enddo
      Call Tridiag(AM,A0,AP,S,X3,N,Nn)
```

There are several alternative algorithms of 1st order that can be used.

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 is repeatedly solved with the updated $X_j(i)$ until the solution for the $X_k(i)$ has converged here defined as

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

where δX is the difference in values of X between succesive iterations.

Solving structure equations give X_i

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 $X(1,i)$ and Z

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

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

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

$$E(3,i) = [T_{i+1} - T_i] - \frac{1}{2}\left[\left(\frac{dT}{dr^2}\right)_i + \left(\frac{dT}{dr^2}\right)_{i+1}\right]\left[r_{i+1}^2 - r_i^2\right]$$

$$E(4,i) = \log\left(\frac{T_{i+1}}{T_i}\right) - \frac{1}{2}\left[\nabla_{i+1} - \nabla_i\right]\log\left(\frac{P_{i+1}}{P_i}\right)$$

The equations are satisfied when $E(k,i) = 0$

The $E(k,i)$ depend on the variables at $V(j,i), V_0(j,i), V(j,i+1), V_0(j,i+1)$, $j = 1, 4$. We iterate to find the values of the $V(j,i)$ 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

$$A(k,j,i)\,\delta V(j,i) = -E(k,i)$$

where A is a block diagonal matrix, the blocks being 8 x 4. This system is readily solved by elimination of the first 2 columns in each block, diagonalisation of the 4 x 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 is obtained.

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

Parameters for comparison models

For all values of X_1, Z the initial abundances were taken as

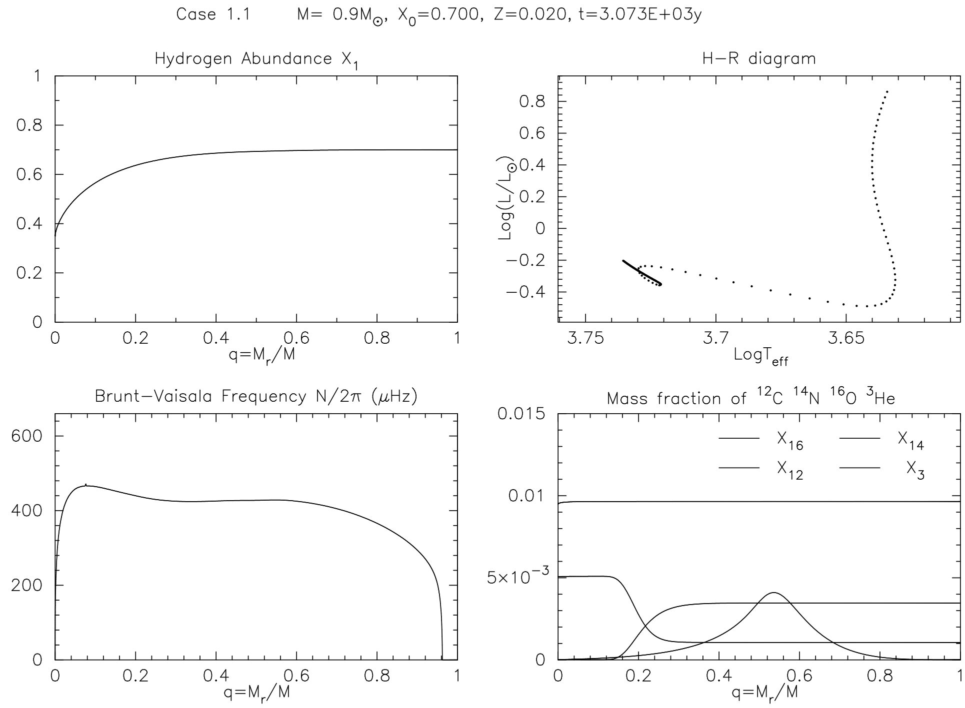
$X_3 = 10^{-5}, \quad X_{12} = 0.173285\,Z, \quad X_{14} = 0.053152\,Z, \quad X_{16} = 0.482273\,Z$

$X_4 = 1 - X_1 - Z$, all other $X_k = 0$

All models started on the pre main sequence with a (nominal) initial radius $R_i = 5R_\odot$ except model 1.4 where $R_i = 10R_\odot$. The mesh was $N = 2000$ in all cases; $i = 0, 2001$ with the photosphere intercalated.

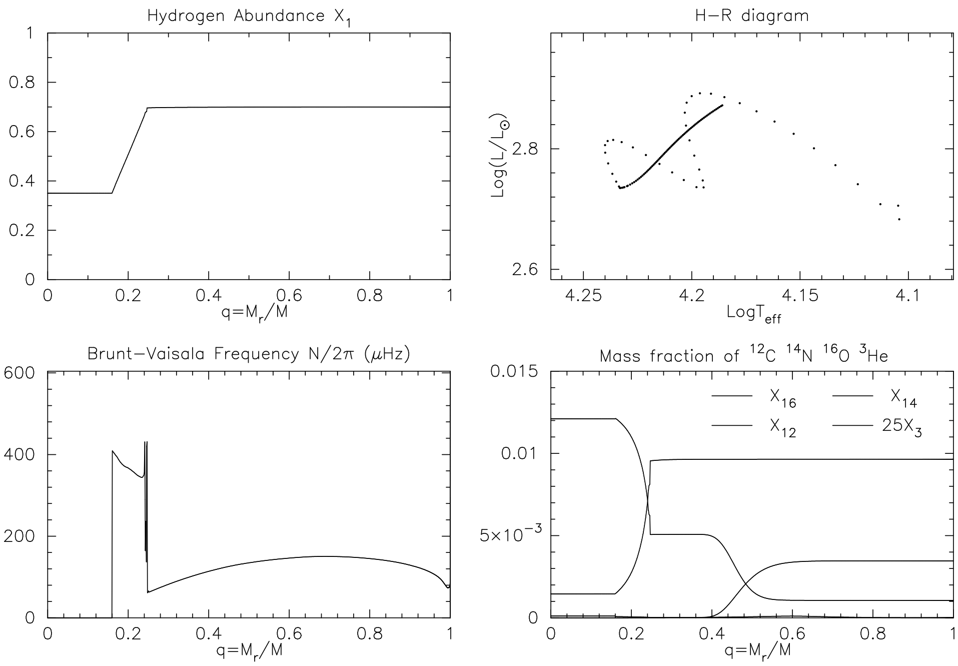
Results from staroxNACRE17

case	Age	$R/R_\odot$	$L/L_\odot$	T_{eff}	T_{7c}	ρ_c	X_c	M_c/M	R_e/R
1.1	6674	0.8926	0.6259	5439	1.446	151.8	0.3500	0.0000	0.6964
1.2	101.5	1.1483	1.778	6225	1.576	86.84	0.6900	0.0076	0.8292
1.3									
1.4	8.292	1.8623	15.64	8419	1.900	49.19	0.6994	0.1077	0.9917
1.5	1197	3.6520	23.32	6644	2.801	131.8	0.0101	0.0635	0.9854
1.6	14.46	1.8552	101.6	13468	2.487	43.17	0.6900	0.2118	0.9939
1.7	55.60	3.8708	744.9	15342	2.838	19.76	0.3500	0.1597	0.9929

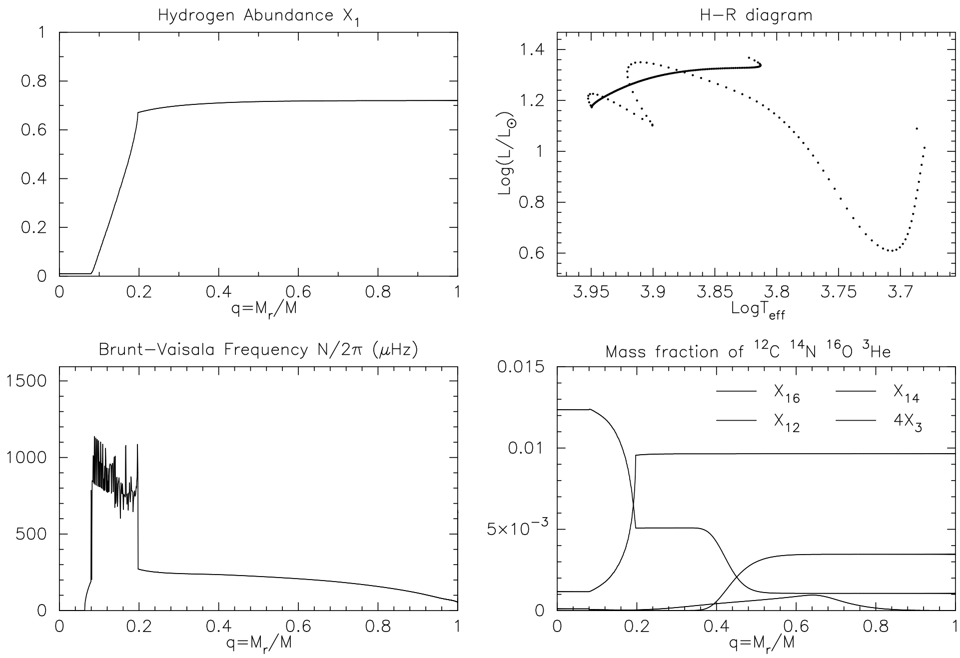


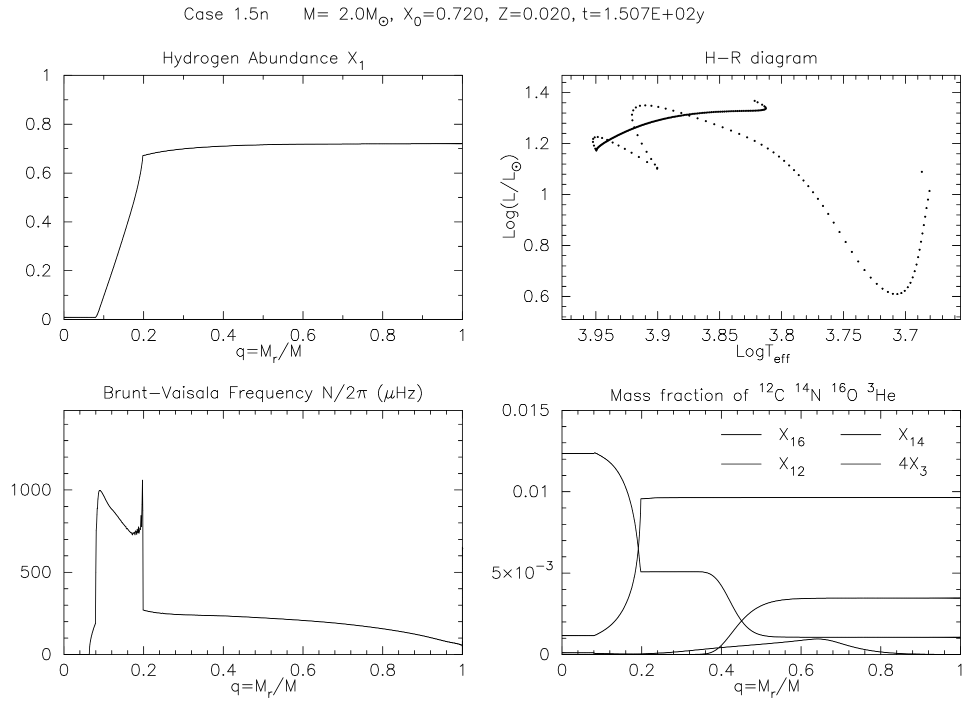
Case 1.1 M= 0.9M⊙, X0=0.700, Z=0.020, t=3.073E+03y
Hydrogen Abundance X1
q=Mr/M
H–R diagram
Log(L/L⊙)
LogTeff
Brunt–Vaisala Frequency N/2π (μHz)
q=Mr/M
Mass fraction of 12C 14N 16O 3He
X16
X14
X12
X3
q=Mr/M

Case 1.7 M= 5.0M$_\odot$, X_0=0.700, Z=0.020, t=6.514E+03y



Case 1.5 M= $2.0M_{\odot}$, X_0=0.720, Z=0.020, t=1.507E+02y




Case 1.5n M= 2.0M⊙, X0=0.720, Z=0.020, t=1.507E+02y
Hydrogen Abundance X1
q=Mr/M
H-R diagram
Log(L/L⊙)
LogTeff
Brunt-Vaisala Frequency N/2π (μHz)
q=Mr/M
Mass fraction of 12C 14N 16O 3He
X16
X14
X12
4X3
q=Mr/M

Output File

eg $m0.90Z.020X0.350$ for $M = 0.90M_{\odot}, Z = 0.020, Xc = 0.350$

```
      open(1, file='m0.90Z.020X0.350')
      read(1,*) N, Gee, Rs, Ms, dLro2, dLP2, Xc, X0, Z, LLs, Te, age6,
     1              qc, xe, alpha, tau
      do i=0,N
           read(,* ) j, x(i), q(i), P(i), rho(i), Gamma1(i), D(i), dq(i), L(i),
     1             T(i), X1(i), X3(i), X4(i), X12(i), X14(i), X16(i)
      enddo
c     This is evolutionary sequence leading to output model
      read(1,*)  im, Ms, X0, Z, age6, alpha, tau
      do i=1,im
         read(1,*)  j, age(i), Tei(i), Li(i), X1c(i), Ri(i), rhoc(i), Tc(i), qci(i), xei(i)
      enddo
      close(1)
```

Rs=photospheric radius, X0=initial X1, LLs=L/$L_{\odot}$, age6=age/10^6y

x=r/Rs, q=Mr/Ms, dq(i)=q(i)-q(i-1), $D(i) = 1/\Gamma_1 - d\log\rho/d\log P$

Ms is mass, Rs the photospheric radius, dLro2, dLP2 are second derivatives at x=0 useful for determining oscillation frequencies, Xc is central hydrogen abundance, X0 the initial hydrogen abundance, LLs=L/$L_{\odot}$, Te the effective temperature, age6 the age in units of 10^6 years, qc=Mc/Ms the fractional core mass, xe=re/Rs the fractional radius at base of the deepest convective envelope, alpha the mixing length parameter and tau the surface optical depth.

Results from staroxNACRE17

case	Age	$R/R_\odot$	$L/L_\odot$	T_{eff}	T_{7c}	ρ_c	X_c	M_c/M	R_e/R
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1.7	55.60	3.8708	744.9	15342	2.838	19.76	0.3500	0.1597	0.9929

with movable overshoot boundary

1.5n	1200	3.6630	23.32	6634	2.799	131.4	0.0103	0.0636	0.9850

fully implicit

1.1	6733	0.8933	0.6281	5442	1.449	152.2	0.3500	0.0000	0.6965

full mix con core

1.1	6670	0.8926	0.6259	5439	1.446	151.8	0.3500	0.0000	0.6964

time centred (unstable)

1.1	7018	0.8983	0.6382	5449	1.450	156.1	0.3500	0.0000	0.6959

dX1dt-2000

1.1	6862	0.8936	0.6274	5439	1.448	151.7	0.3500	0.000	00.6962

dX1dt-1000

1.1	6862	0.8938	0.6274	5439	1.448	151.7	0.3500	0.0000	0.6962

dX1dt-500

1.1	6863	0.8944	0.6273	5437	1.448	151.7	0.3500	0.0000	0.6962

dX1dt-2000

1.1	6862	0.8936	0.6274	5439	1.448	151.7	0.3500	0.0000	0.6962

dX1dt/2-2000

1.1	6798	0.8934	0.6277	5441	1.448	152.0	0.3500	0.0000	0.6963

dX1dt/4-2000

1.1	6769	0.8933	0.6279	5441	1.448	152.1	0.3500	0.0000	0.6964

dX1dt/4-500

1.1	6770	0.8941	0.6277	5439	1.448	152.1	0.3500	0.0000	0.6964

dX11dt/4-2000

1.1	6764	0.8933	0.6278	5441	1.448	152.1	0.3500	0.0000	0.6964