### ASTEC

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### **Basic numerical scheme**

$$\begin{split} &\frac{\partial z_l}{\partial x} = f_l(x; y_i; t) , \qquad l = 1, \dots I_1 \quad \text{Type I} \\ &\frac{\partial z_p}{\partial x} = f_p(x; y_i; t) + \sum_{i=1}^{I} \Lambda_{pi}(x; y_j; t) \frac{\partial y_i}{\partial t} , \qquad p = I_1 + 1, \dots I_1 + I_2 \quad \text{Type II} \\ &\frac{\partial z_u}{\partial t} = f_u(x; y_i; t) , \qquad u = I_1 + I_2 + 1, \dots I_1 + I_2 + I_3 \quad \text{Type III} \\ &z_i = z_i(x; y_j; t) , \qquad i = 1, \dots I , \\ &g_\alpha(x_1; y_i(x_1); \lambda_k) = 0 , \qquad \alpha = 1, \dots, KA , \\ &g_\beta(x_2; y_i(x_2); \lambda_k) = 0 , \qquad \beta = KA + 1, \dots, KA + KB . \end{split}$$

Subroutine tnrkt

## Treatment of diffusion

**Basic equation** 

$$\frac{\partial X_i}{\partial t} = \frac{\partial}{\partial m} \left( \mathcal{D}_i \frac{\partial X_i}{\partial m} \right) + \frac{\partial}{\partial m} (\mathcal{V}_i X_i) + \mathcal{R}_i \,,$$

introduce

$$Y_i = \mathcal{D}_i \frac{\partial X_i}{\partial m} + \mathcal{V}_i X_i$$
;

Then

$$\frac{\partial X_i}{\partial m} = \mathcal{D}_i^{-1} Y_i - \mathcal{D}_i^{-1} \mathcal{V}_i X_i ,$$
  
$$\frac{\partial Y_i}{\partial m} = \frac{\partial X_i}{\partial t} - \mathcal{R}_i ,$$

is on tnrkt form

### Discretization

- Second-order spatially centred differences
- Time-centred differences in evolution equation for H
- Backwards differences for other elements, in general, and in energy equation (for stability)

### Implementation details: Mesh

The scheme for defining the mesh is broadly as described by CD82; however, a very dense mesh is used near the boundary of a possible convective core.

Most calculations for CoRoT comparison used 601 points (between centre and photosphere). However, also tests of effect of increasing number of meshpoints.

### **Distribution of meshpoints**

Define mesh  $\{x_n\}, n = 1, ..., N$  to be uniform in a suitably defined function  $\xi(x)$ ; if  $\xi(x_1) = 1$ and  $\xi(x_N) = N$ , the mesh is defined such that  $\xi(x_n) = n, n = 1, ..., N$ .

Compute

$$\xi(x) = 1 + \lambda \int_{x_1}^x g(x) \mathrm{d}x \; ,$$

where  $\lambda$  is a constant that is chosen such that  $\xi(x_N) = N$ .

$$g(x) = \begin{cases} \frac{w_0^2}{(x_N - x_1)^2} + \sum_{i=1}^6 w_i^2 s_i^{-2} \left(\frac{\mathrm{d}\eta_i}{\mathrm{d}x}\right)^2 \\ + s_7^{-2} w_7^2 \left[ \left(\frac{\mathrm{d}\eta_7}{\mathrm{d}x}\right)^2 + a_7^2 \eta_7^2 \left(\frac{\mathrm{d}^2\eta_7}{\mathrm{d}x^2}\right)^2 \right] + \Psi(x) \end{cases}^{1/2}$$

Here  $\eta_1 = r$ ,  $\eta_2 = \log p$ ,  $\eta_3 = \log T$ ,  $\eta_4 = \log L$ ,  $\eta_5 = \log r_X$ ,  $\eta_6 = \log(10-5+X_3)$ , and  $\eta_7 = \nabla - \nabla_{ad}$ .

 $s_i = \max(\eta_i(x)) - \min(\eta_i(x)) .$ 

 $\Psi(x)$  allows adding points in critical regions, such as edge of convective core.

## Implementation details: Pulsation mesh

Mesh reset for pulsation calculation, depending on desired modes (distribution largely determined by asymptotic behaviour of eigenfunctions).

Let 
$$x = r/R$$
,  $\hat{c}^2 = (R/GM)c^2$ ,  $\hat{N}^2 = (R^3/GM)N^2$ .

$$g(x) = \left[1 + w_1^2 \hat{c}^{-2} + w_2^2 \frac{|\hat{N}|^2}{x^2} + w_3^2 \left(\frac{d\ln p}{dx}\right)^2\right]^{1/2}$$

Note that if term in  $w_1$  dominates, mesh is uniform in

$$\int_0^x \frac{\mathrm{d}x}{\widehat{c}} \; ,$$

i.e., acoustical radius, as is appropriate for acoustic modes.

Additional points are added near discontinuities in density.

#### 1.3 M-



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## Implementation details: Timestep

The timestep is set based on relative (or  $\log_{10}$ ) changes in several quantities being limited to be below a specified limit  $\Delta y_{max}$ .

Changes in the hydrogen abundance in a convective core are scaled by a factor 5, to compensate for the rather crude numerical treatment of the core composition. As a result, more timesteps are used in models with a convective core.

In the present case, typically 200 steps are required to reach exhaustion of hydrogen at the centre, in models with a convective core, and 30 - 40 steps in a model without (this small number is also a consequence of the crude treatment of the nuclear network).

## Implementation details: equation of state

OPAL 2001 tables, for the appropriate value of Z (= 0.02 or 0.01). Using the OPAL interpolation scheme.

### Implementation details: opacity

OPAL 1996 tables, with Alexander low-temperature values. Houdek interpolation scheme. The heavy-element abundance is taken to be the initial value, regardless of the changes due to nuclear reactions.

(In models with diffusion and settling, these effects on heavy elements are decoupled from the nuclear changes in composition, for now. The modified heavy-element abundance is used for the opacity but not, usually, for interpolated equations of state.)

### Implementation details: nuclear reactions

For Toulouse comparison: nuclear reaction parameters generally from Bahcall & Pinsonneault (1995).

NACRE now implemented. Corrected 21/10/05!

Salpeter weak screening.

# Implementation details: treatment of convection

Böhm-Vitense (1958) mixing-length treatment, probably with Henyey et al. (1965) detailed parameters. (The specification of these parameters seems a little uncertain.)

Turbulent pressure is not included.

## Implementation details: treatment of atmosphere

Integration of hydrostatic equation assuming the grey Eddington T( $\tau$ ) relation: T = T<sub>eff</sub> [3/4\*( $\tau$  + 2/3)]<sup>0.25</sup>, starting at  $\tau$  = 0.01 and matching where T = T<sub>eff</sub> ( $\tau$  = 2/3).

Note that there are potential problems with the treatment of radiation pressure in the atmosphere, certainly for relatively massive (and hot) stars.)

# Implementation details: initial model, chemical evolution

The models start from the ZAMS (PMS evolution has been used in the code, but not tested with care).

Chemical evolution is integrated with the general solution of the structure and evolution equations (tnrkt).

A separate treatment is used for the chemical evolution of the convective core, using the averaged reaction rates. This is carried out in parallel with the Henyey iteration, although occasionally with fixes to ensure convergence (freezing the properties of the core).

CN part of the CNO cycle is assumed to be in nuclear equilibrium at all times; initial <sup>14</sup>N abundance includes also the original <sup>12</sup>C abundance. The conversion of <sup>16</sup>O into <sup>14</sup>N is taken into account. The initial abundances of <sup>14</sup>N and <sup>16</sup>O, relative to the heavy-element abundance, are 0.2337 and 0.5154. (May well need to be changed, to meet specifications.)

## Implementation details: treatment of <sup>3</sup>He

Original models (for Toulouse):

<sup>3</sup>He is assumed to be in nuclear equilibrium at all times.

Recent modelling (and always used in solar case):

Set ZAMS <sup>3</sup>He abundance by evolving abundance for time  $\tau_3$  at constant conditions, starting from initially constant abundance.

Typical value (for solar models):  $\tau_3 = 5 \text{ \pounds } 10^7$  years

Also try  $\tau_3$  = 10<sup>7</sup> years for 0.9 M– model.

### Detailed test of Case 1.1

 $0.9 \text{ M} - X_c = 0.35$ 





















### Physics comparisons

Evaluate physics (EOS, opacity, energy-generation rate, rate of composition change, ..., at fixed T,  $\rho$ , X<sub>i</sub>

Examples: comparing CESAM and CLES with ASTEC, showing, e.g.,

 $ln(\kappa_{ASTEC}(\rho_{CESAM}, T_{CESAM}, ...)/\kappa_{CESAM})$ 















### CLES, Case 1.1



