The modeling of microscopic diffusion in the Geneva evolution code

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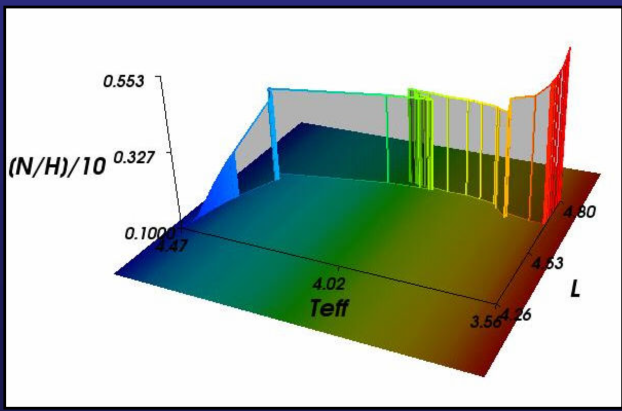
Overview

- Introduction
- Modeling of microscopic diffusion
- Numerical methods
- Application to solar-type stars
- Conclusion

Introduction

- Models of massive stars
  - Grids of stellar models at various metallicities
    (Maeder & Meynet 1987; Schaller et al. 1992; Schaerer et al. 1993; Charbonnel et al. 1993; Meynet et al. 1994; Mowlavi et al. 1998)
- Inclusion of rotation
  - Surface enrichments of massive stars
  - The B/R ratio
  - Nature of the supernova progenitor
  - Stellar yields



Introduction

- Models of solar-type stars
  - Grids for low mass stars
    (Charbonnel et al. 1996, 1999)
  - Solar models
    (Lebreton & Maeder 1986, 1987; Charbonnel et al. 1994; Richard et al. 1996, 2004)
  - Stellar models of asteroseismic targets
    (Eggenberger et al. 2004, 2005, 2006)
  - Input physics:
    - Equation of state: MHD and OPAL
    - Inclusion of microscopic diffusion

Modeling of microscopic diffusion

- The diffusion equation

$$\rho\frac{\partial c}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\rho D\frac{\partial c}{\partial r} - r^2\rho c V\right) - \lambda\rho c$$

- Chemical elements:
  - 15 isotopes:
    H, ^{3}He, ^{4}He, ^{12}C, ^{13}C, ^{14}N, ^{15}N, ^{16}O, ^{17}O, ^{18}O,
    ^{20}Ne, ^{22}Ne, ^{24}Mg, ^{26}Mg, ^{26}Mg
  - Changes due to diffusion / nuclear reactions
  - λ : only for lithium and beryllium
- Microscopic diffusion:
  - Routines of the Toulouse-Geneva version of the code
  - Radiative acceleration is neglected

Modeling of microscopic diffusion

- The Chapman-Enskog method (Chapman & Cowling 1970)
  - Boltzmann equation
  - Expansion of f in a series of decreasing order

$$\frac{\partial c_i}{\partial t} = D'_{1i}\frac{\partial^2 c_i}{\partial m_r^2} + \left(\frac{\partial D'_{1i}}{\partial m_r} - V'_{1i}\right)\frac{\partial c_i}{\partial m_r} - \left(\frac{\partial V'_{1i}}{\partial m_r} + \lambda_i\right)c_i$$

$$D'_{1i} = \left(4\pi\rho r^2\right)^2\left(D_{\rm turb} + D_{1i}\right)$$

$$V'_{1i} = \left(4\pi\rho r^2\right)V_{1i}$$

$$V_{1i} = -D_{1i}\left[\left(A_i - \frac{Z_i}{2} - \frac{1}{2}\right)\left(\frac{m_H}{kT}\frac{Gm_r}{r^2}\right) - \alpha_{1i}\nabla\ln T\right]$$

Modeling of microscopic diffusion

- Computation of the diffusion coefficients
  - Formalism of Paquette et al. (1986)

$$D_{st} = \frac{3E}{2nm(1-\Delta)} \quad \text{and} \quad \alpha_{st} = \frac{5C(x_s S_s - x_t S_t)}{x_s^2 Q_s + x_t^2 Q_t + x_s x_t Q_{st}}$$

  - Collision integrals:

$$\Omega_{st}^{(ij)} = \left(\frac{kT}{2\pi m M_s M_t}\right)^{1/2} \int_0^\infty e^{-g^2} g^{2j+3} \phi_{st}^{(i)} \mathrm{d}g$$

$$\phi_{st}^{(i)} = 2\pi \int_0^\infty (1-\cos^i \chi_{st}) b \mathrm{d}b \quad \text{and} \quad \chi_{st} = \pi - 2\int_{r_{st}^{\min}}^\infty b \mathrm{d}r \left\{ r^2 \left[1 - \frac{b^2}{r^2} - \frac{V_{st}(r)}{g^2 kT}\right]^{1/2} \right\}^{-1}$$

with r_{st}^{min} defined by: $1 - \frac{b^2}{\left(r_{st}^{\min}\right)^2} - \frac{V_{st}\left(r_{st}^{\min}\right)}{g^2 kT} = 0$

Modeling of microscopic diffusion

- Computation of the collision integrals
  - Static screened potential:

$$V_{st}(r) = Z_s Z_t e^2 \frac{e^{-r/\lambda}}{r} \quad \text{with} \quad \lambda_D = \left(\frac{kT}{4\pi e^2 \sum_i n_i Z_i^2}\right)^{1/2}, \quad \lambda_i = \left(\frac{3}{4\pi n_i}\right)^{1/3}$$

  - Analytic fits:
    - Dimensionless collision integrals

$$F_{st}^{(ij)} = \frac{\Omega_{st}^{(ij)}}{\epsilon_{st}} \quad \text{with} \quad \epsilon_{st} = \pi \left(\frac{Z_s Z_t e^2}{2kT}\right)^2 \left(\frac{kT}{2\pi m M_s M_t}\right)^{1/2}$$

    - Independent variable

$$\psi_{st} = \ln[\ln(1+\gamma_{st}^2)] \quad \text{where} \quad \gamma_{st} = \frac{4kT\lambda}{Z_s Z_t e^2}$$

Modeling of microscopic diffusion

- Computation of the collision integrals
  - Analytic fits: 3 regions:

    i) $-7.0 \leq \psi_{st} \leq 3.0$

    ii) $3.0 \leq \psi_{st} \leq 4.0$

    iii) $\psi_{st} \geq 4.0$

  - Example:

$$\ln F_{st}^{(22)} = d_{1n}[\psi_{st}(n+1) - \psi_{st}]^3 + d_{2n}[\psi_{st} - \psi_{st}(n)]^3 + d_{3n}[\psi_{st}(n+1) - \psi_{st}] + d_{4n}[\psi_{st} - \psi_{st}(n)]$$

TABLE 4

SPLINE COEFFICIENTS (REPULSIVE POTENTIAL): $l = 1$–4

n	d_{1n}	d_{2n}	d_{3n}	d_{4n}
1	1.18229E-02	-2.38458E-02	-2.55112E+01	-2.47319E+01
2	-2.38458E-02	-1.45794E-02	-2.47319E+01	-2.39583E+01
3	-1.45794E-02	-1.76226E-02	-2.39583E+01	-2.31882E+01
4	-1.76226E-02	-1.73748E-02	-2.31882E+01	-2.24223E+01
5	-1.73748E-02	-1.79780E-02	-2.24223E+01	-2.16606E+01
6	-1.79780E-02	-1.83439E-02	-2.16606E+01	-2.09032E+01
7	-1.83439E-02	-1.87580E-02	-2.09032E+01	-2.01502E+01
8	-1.87580E-02	-1.91359E-02	-2.01502E+01	-1.94017E+01
9	-1.91359E-02	-1.94807E-02	-1.94017E+01	-1.86579E+01
10	-1.94807E-02	-1.98074E-02	-1.86579E+01	-1.79186E+01
11	-1.98074E-02	-2.00758E-02	-1.79186E+01	-1.71842E+01
12	-2.00758E-02	-2.02617E-02	-1.71842E+01	-1.64545E+01
13	-2.02617E-02	-2.04080E-02	-1.64545E+01	-1.57298E+01
14	-2.04080E-02	-2.04344E-02	-1.57298E+01	-1.50099E+01
15	-2.04344E-02	-2.03360E-02	-1.50099E+01	-1.42949E+01
16	-2.03360E-02	-2.00828E-02	-1.42949E+01	-1.35848E+01
17	-2.00828E-02	-1.96388E-02	-1.35848E+01	-1.28796E+01
18	-1.96388E-02	-1.89603E-02	-1.28796E+01	-1.21790E+01
19	-1.89603E-02	-1.79946E-02	-1.21790E+01	-1.14830E+01
20	-1.79946E-02	-1.66781E-02	-1.14830E+01	-1.07913E+01
21	-1.66781E-02	-1.49334E-02	-1.07913E+01	-1.01036E+01
22	-1.49334E-02	-1.26670E-02	-1.01036E+01	-9.41952E+00
23	-1.26670E-02	-9.76488E-03	-9.41952E+00	-8.73845E+00
24	-9.76488E-03	-6.08817E-03	-8.73845E+00	-8.05874E+00
25	-6.08817E-03	-1.46668E-03	-8.05874E+00	-7.38248E+00
26	-1.46668E-03	4.30758E-03	-7.38248E+00	-6.70557E+00
27	4.30758E-03	1.14919E-02	-6.70557E+00	-6.02763E+00
28	1.14919E-02	2.04026E-02	-6.02763E+00	-5.34694E+00
29	2.04026E-02	3.14302E-02	-5.34694E+00	-4.66134E+00
30	3.14302E-02	4.50547E-02	-4.66134E+00	-3.96821E+00
31	4.50547E-02	6.18616E-02	-3.96821E+00	-3.26426E+00
32	6.18616E-02	8.25526E-02	-3.26426E+00	-2.54546E+00
33	8.25526E-02	1.07839E-01	-2.54546E+00	-1.80685E+00
34	1.07839E-01	1.38897E-01	-1.80685E+00	-1.04234E+00
35	1.38897E-01	1.76234E-01	-1.04234E+00	-2.44487E-01
36	1.76234E-01	2.20387E-01	-2.44487E-01	5.95659E-01
37	2.20387E-01	2.70814E-01	5.95659E-01	1.48670E+00
38	2.70814E-01	3.24880E-01	1.48670E+00	2.44673E+00
39	3.24880E-01	3.76096E-01	2.44673E+00	3.48274E+00
40	3.76096E-01	4.11895E-01	3.48274E+00	4.60901E+00
41	4.11895E-01	4.12194E-01	4.60901E+00	5.83413E+00
42	4.12194E-01	3.52178E-01	5.83413E+00	7.15818E+00
43	3.52178E-01	2.14860E-01	7.15818E+00	8.56675E+00
44	2.14860E-01	1.56932E-02	8.56675E+00	1.00269E+01
45	1.56932E-02	-1.84529E-01	1.00269E+01	1.14908E+01
46	-1.84529E-01	-3.17740E-01	1.14908E+01	1.29104E+01
47	-3.17740E-01	-3.51788E-01	1.29104E+01	1.42538E+01
48	-3.51788E-01	-2.86379E-01	1.42538E+01	1.55127E+01
49	-2.86379E-01	-2.68214E-01	1.55127E+01	1.67029E+01
50	-2.68214E-01	1.34107E-01	1.67029E+01	1.78287E+01

Modeling of microscopic diffusion

- Summary
  - Computation of the collision integrals using the analytic fits of Paquette et al. (1986)
  - Determination of the diffusion coefficients D_{1i} and α_{1i}, as well as the diffusion velocity V_{1i}
  - The diffusion equation is then solved

Numerical Methods

- Crank-Nicholson finite differences

$$\frac{\partial c}{\partial t} = D\,\frac{\partial^2 c}{\partial r^2} + E\,\frac{\partial c}{\partial r} + F\,c$$

  - K shells: $\mathbf{C} = (c_1;\ldots;c_K)$ with $S = r_j - r_{j-1}$ and $P = r_{j+1} - r_j$

$$c_{j-1} = c_j - S\left(\frac{\partial c}{\partial r}\right)_j + \frac{S^2}{2}\left(\frac{\partial^2 c}{\partial r^2}\right)_j \qquad \left(\frac{\partial c}{\partial r}\right)_j = A_1 c_{j-1} + B_1 c_j + C_1 c_{j+1}$$

$$c_{j+1} = c_j + P\left(\frac{\partial c}{\partial r}\right)_j + \frac{P^2}{2}\left(\frac{\partial^2 c}{\partial r^2}\right)_j \qquad \left(\frac{\partial^2 c}{\partial r^2}\right)_j = A_2 c_{j-1} + B_2 c_j + C_2 c_{j+1}$$

  - Diffusion equation:

$$\frac{\partial c_j}{\partial t} = (DA_2 + EA_1)c_{j-1} + (DB_2 + EB_1 + F)c_j + (DC_2 + EC_1)c_{j+1}$$

in vector form: $$\frac{\partial \mathbf{C}}{\partial t} = \mathbf{MC}$$

Numerical Methods

- Implicit finite elements
  - Method used by Glowinsky and Angrand (Schatzman et al. 1981)

$$v_i(m_r) = \begin{cases} \nearrow \frac{m_r - m_{i-1}}{m_i - m_{i-1}} & \text{if } m_r \in [m_{i-1}, m_i] \\ \rightarrow \frac{m_r - m_i}{m_i - m_{i+1}} & \text{if } m_r \in [m_i, m_{i+1}] \\ \searrow 0 & \text{if } m_r \notin [m_{i-1}, m_{i+1}] \end{cases}$$

  - Diffusion equation: $$\int_{M_1}^{M_2} \frac{\partial c}{\partial t} v_i \mathrm{d}m + \int_{M_1}^{M_2} D' \frac{\partial c}{\partial m}\frac{\partial v_i}{\partial m}\mathrm{d}m - \int_{M_1}^{M_2} V' c \frac{\partial v_i}{\partial m}\mathrm{d}m$$

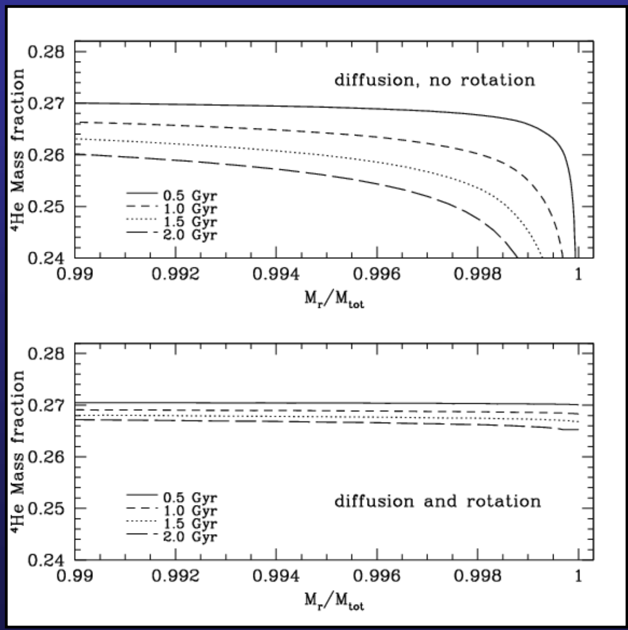
$$- \int_{M_1}^{M_2} \lambda c v_i \mathrm{d}m + \frac{\partial}{\partial t}(cM_{zc_1}) - \frac{\partial}{\partial t}(cM_{zc_2}) = 0$$

  - with $c = \Sigma_j\ C_j\ v_j$:

$$\frac{\partial}{\partial t}(M_{j,i}C_j) + N_{j,i}C_j - P_{j,i}C_j + \frac{\partial}{\partial t}(C_1 M_{zc_1}) - \frac{\partial}{\partial t}(C_K M_{zc_2}) = 0$$

Application to solar-type stars

- Stars with a shallow convective envelope
  - Exemple: η Bootis (G0 IV)
  - Rotation counteracts the effects of microscopic diffusion in the external layers



Carrier et al. 2005, A&A, 434, 1085

Conclusion

- Summary
  - Diffusion routines of the Toulouse-Geneva code
  - Chapman-Enskog method is used
  - Collision integrals calculated from the analytic fits of Paquette et al. (1986)
  - Numerical methods: Crank-Nicholson finite differences or Implicit finite elements
- Future perspectives
  - Models of solar-type stars including microscopic diffusion and a comprehensive treatment of rotation
    - Internal gravity waves (Talon et al. 2002; Charbonnel & Talon 2005)
  - Inclusion of magnetic field:
    - Magnetic instabilities (Maeder & Meynet 2004; Braithwaite & Spruit 2005; Eggenberger et al. 2005; Brun & Zahn 2006)
    - Secular torque (Charbonneau & Mac Gregor 1993; Mathis & Zahn 2005)