Diffusion in Clés

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Diffusion in Clés
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Diffusion in Clés
1. Chemical evolution

1. Chemical evolution

$$\frac{dX_i}{dt} = \sum_j R_{ij} - \frac{1}{\rho r^2}\frac{\partial}{\partial r}\left(r^2 \rho X_i w_i\right)$$

Nuclear reaction

Diffusion velocity

Diffusion in Clés
1. Chemical evolution

Chemical evolution in convective regions

2 different approaches : Turbulent diffusion

Instantaneous mixing → CLES

- X_i independent of r
- evolution governed by :

$$m_c \frac{dX_i}{dt} = \int_{m_1}^{m_2} \sum_j R_{ij}\, dm - \left(4\pi r^2 \rho X_i w_i\right)_2 + \left(4\pi r^2 \rho X_i w_i\right)_1$$

Diffusion in Clés
2. Diffusion theory

2. Diffusion theory of Thoul et al. (1994)

$$\frac{dP_i}{dr} + \rho_i g - \rho_{ei} E = \sum_{j\neq i} K_{ij}\left[(w_j - w_i) + 0.6\,(x_{ij} r_i - y_{ij} r_j)\right] \quad \Rightarrow \quad n+1$$

$$\frac{5}{2} n_i k \frac{dT}{dr} = \sum_{j\neq i} K_{ij}\left\{\frac{3}{2} x_{ij}(w_i - w_j) - y_{ij}\left[1.6 x_{ij}(r_i + r_j) + Y_{ij} r_i - 4.3 x_{ij} r_j\right]\right\} - 0.8 K_{ii} r_i \quad \Rightarrow \quad n+1$$

$$\sum_i m_i n_i w_i = 0 \quad \text{(local mass conservation)} \quad \Rightarrow \quad +1$$

$$\sum_i q_i n_i w_i = 0 \quad \text{(current neutrality)} \quad \Rightarrow \quad +1$$

q_i → $Z_i e$

i,j : all involved chemical species including electrons → n + 1

Diffusion in Clés
2. Diffusion theory

- *2n + 4* equations
- *2n + 4* unknowns :
  - *n+1* w_i
  - *n+1* r_i
  - *g* and *E*

$$\Rightarrow \quad w_i = \sum_j a_{ij} \frac{dX_j}{dr} + a_P \frac{d\ln P}{dr} + a_T \frac{d\ln T}{dr}$$

j : all involved chemical species, excluding electrons

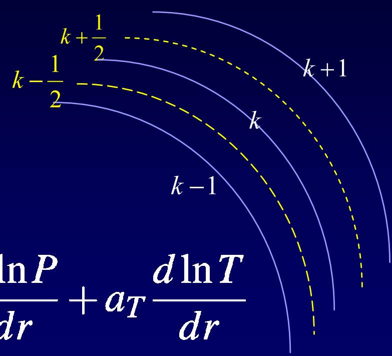
a_{ij}, a_P, a_T = fct (X, $\overline{Z}$, …)

3. Implementation

Overwiew

Diffusion implemented for a dozen species

- Computing diffusion coefficients : a_{ij} a_P, a_T = fct (… , $\overline{Z}$, …) :
  - mean charge : computed from the Saha equations
  - a_{ij}, a_P, a_T : computed from the Burgers equations
- Diffusion-induced abundance variations
  - computed apart from nuclear burning and convection effects $\Rightarrow$ problem for Li, Be and B



Discretization

$$\frac{dX_i}{dt} = -\frac{1}{\rho r^2}\frac{\partial}{\partial r}(r^2 \rho X_i w_i) \qquad w_i = \sum_j a_{ij}\frac{dX_j}{dr} + a_P\frac{d\ln P}{dr} + a_T\frac{d\ln T}{dr}$$

$$\frac{X_{ik} - X_{ik}^0}{\delta t} = -\frac{(4\pi r^2 \rho X_i w_i)_{k+1/2} - (4\pi r^2 \rho X_i w_i)_{k-1/2}}{m_{k+1/2} - m_{k-1/2}}$$

$$w_{i,k+1/2} = \frac{\sum_j a_{ij,k+1/2}(X_{j,k+1} - X_{jk}) + a_{P,k+1/2}(\ln P_{k+1} - \ln P_k) + a_{T,k+1/2}(\ln T_{k+1} - \ln T_k)}{r_{k+1} - r_k}$$

with $X_{ik}^0 = X_{ik}$ at time $t - \delta t$

$$r_{k+1/2} = (r_k + r_{k+1})/2, \; \ldots$$

Diffusion in Clés
3. Implementation

Numerical technique

- Second members evaluated at time *t* (rather than t - δt)

(as it is the case for the composition variations due to nuclear burning)

- Newton-Raphson algorithm with partial corrections
- Evolution timestep controlled by diffusion.

Diffusion in Clés

The End