Lucio Crivellari
Instituto de Astrofísica de Canarias & Dipartimento di Astronomia – UdS Trieste

Algorithms for the solution of

non-linear and non-local problems

The team:

Eduardo Simonneau (CNRS, Institut d'Astrophysique, Paris)
Octavio Cardona (INAOE, Tonantzintla, Mexico)
Lucio Crivellari (IAC and DAUT)

Numerical algorithms for

Modelling *(stellar atmospheres)*

The Iterative Sequential Approach

The Iteration Factors Method

1988, Astrophys. J., **330**, *415*
1991, Astrphys. J., ***367***, *612*

Solving the RT equation

An implicit integral method to solve selected radiative problems

I. Non-LTE line formation (ApJ, **409**, 830)
II. LTE stellar atmosphere models (ApJ, **429**, 331)
III. Factorization vs. linearization (ApJ, **428**,753)
IV. The case of spherical geometry (ApJ, **489**, 331)

Multilevel line transfer with the implicit integral method, 2002, Astrofizika, **45(5)**, 587

Algorithms for the solution of non-linear and non-local problems

Table of contents

operative vs. operational

From The Oxford Dictionary:

Operative =
characterized by operating or working; active in producing effect

Operationalism =
a theory which accepts only such concepts as can be described in terms of the operations necessary to determine them (P.W. Bridgman, 1927)

1.1 Algorithmic representation of physical systems

Our aim: **an operative description of physical systems**

Basic concepts on structure and representation:

Individual components, **identified and quantified by** ***physical variables***

physical variables $\longleftrightarrow$ **physical magnitudes**

State of a system
described by the values of the fundamental variables

Hierarchy of interactions that shape the structure

The ideal process of dissecting a system into a set of simpler interacting parts allows us to describe the global behaviour of the system in terms of the laws governing its elementary components.

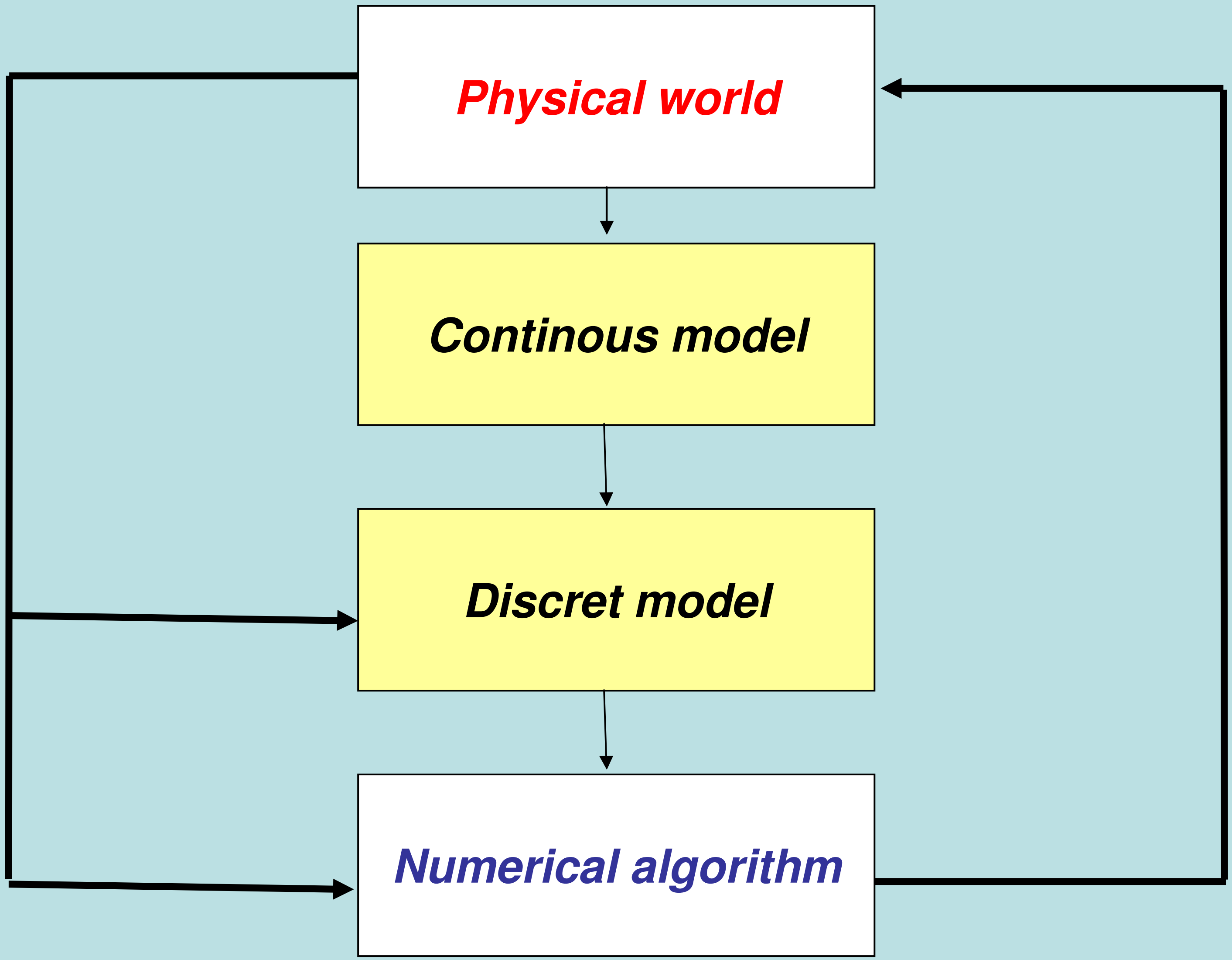
Such a process leads eventually to a

model

- operationally defined -

of our perception of the *physical world*

Modelling is an unparalleled tool for scientific inquiry because,
for its own analytical nature,
It can be easily translated into a mathematical model


Physical world
Continous model
Discret model
Numerical algorithm

1.2 The quest for the optimum algorithm

La physique ne nous donne pas seulement l'ocasión de résoudre des problemes ... Elle nous fait pressentir la solution.
(Henry Poincare)

If the mathematical structure of the algorithm reflects that of the continuous equations

$\Rightarrow$ a performing (*i.e.* *operative*) ***tool***

$\Rightarrow$ an ***image*** of the original physical system

An operative representation of our perception of the physical world

2. The stellar atmosphere problem

The physical system
Stellar atmosphere

The stellar
atmosphere problem

physics:
laws of conservation
transport processes
initial and boundary conditions

non-local and non-linear
problem

structure

modelling

algorithm

The structure of the physical system ''stellar atmosphere'' will be described by the values at each point of the fundamental variables.

These values will be determined by

- ***the relations among the variables***
- ***the constraints imposed by the external conditions***
- ***the internal energy of the system***

The fundamental equations of Stellar Atmosphere Modelling

1. **Constitutive equations:** *Equation of mass conservation*, *Equation of motion*

2. **Equation of state**

3. **The constraint of energy conservation:**

   Energy equations for matter and the radiation field

4. **Transport equations:** *Radiative transfer (RT)*, *Convective transport*

5. **Microscopical description of matter:** *average molecular weight*, *transport coefficients*

LTE: $f(\rho, T)$

Non-LTE: $f(\rho, T, J_\nu)$

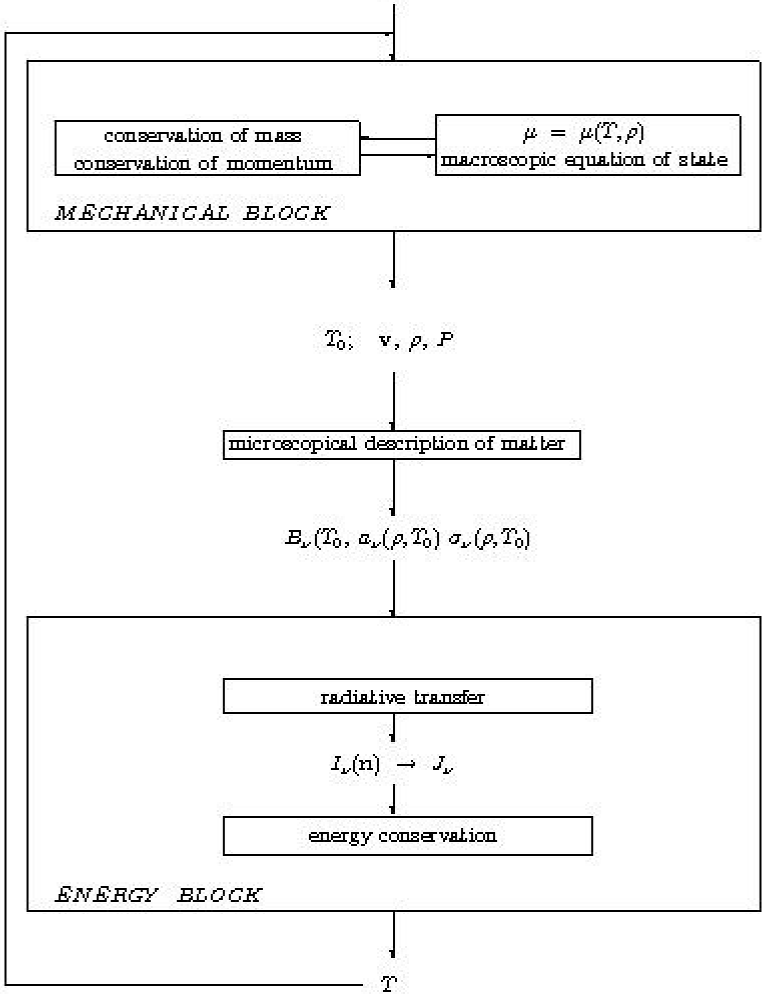


Figure 1: Flow-chart of the natural sequential procedure

The equation of state links the mechanical with the thermodynamical state of the system.

The coefficients μ , η_ν **and** χ_ν

describe the microscopical state; in LTE they are functions of the thermodynamical state only, also of the radiation field in non-LTE.

The transport coefficients η_ν **and** χ_ν

express the dependence, both explicit and implicit, of the energy balance on the solution of the RT equation.

The essential difficulty of the stellar atmosphere problem consists in the fact that all the physical variables interact throughout

***the whole atmosphere*,**

and the local variation of one of them can have an important effect on the

local properties at a great distance.

Via a proper linearization technique, it may be possible to convert the original system into an

equivalent system of linear algebraic equations,

whose matrix will reproduce, for the nature and collocation of its elements, the structure of the initial model.

What looks simple in principle is often infeasible in the practice.

It is well known that the numerical inversion of large or ill-conditioned matrices is a nasty problem.

In a seminal paper von Neumann and Goldstine (1947) showed that when ‘’exact’’ arithmetic is replaced by ‘’approximate' arithmetic, no computing machine can perform faultlessly all the operations, because of the finite number of digits available.

exact $\equiv$ *algebraical and transcendental operations*

approximate $\equiv$ *elementary operations handled by a computer*

At the basis of the complete linearization technique there is the assumption, explicitly stated by Mihalas, that

no variable is more ‘’fundamental’’ than any other, for they all interact

(Mihalas, *Stellar Atmospheres*, 1978, p. 230)

Against this ‘’equalitarian’’ treatment:

i) the different processes are characterized by very different scale;

ii) the strength of the coupling between the different phenomena may vary considerably case by case.

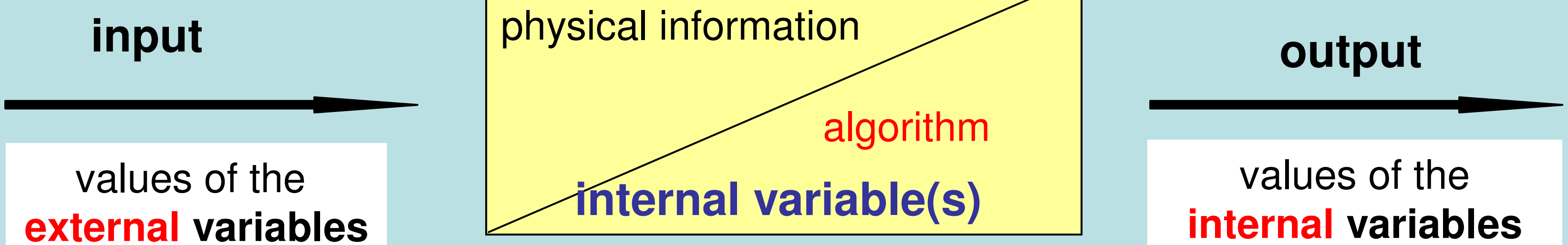
The Iterative Sequential Approach

According to the nature of their mutual interactions the processes are groupped into

elementary blocks

Each block contains an amount of
physical information
that cannot be further reduced

Elementary block



values of the
external variables

values of the
internal variables
solution of the block

atomic self-consistent
physical problem

Simplified stellar atmosphere model:

stationary
homogeneous
plane – parallel
LTE

equation of motion

$$\frac{d\,P(r)}{d\,r} = -\,g\,\rho(r)$$

hydrostatic equilibrium

equation of state

$$P(r) = \frac{k}{m_H\,\mu}\,\rho(r)\,T(r)$$

perfect gas

radiative transfer eq.

$$\mu\,\frac{d\,I_\nu(r;\mu)}{d\,r} = -\,\chi_\nu\,\{I_\nu(r;\mu) - S_\nu[T(r)]\}$$

energy balance eq.

$$\int_0^\infty a_\nu\,J_\nu(r)\,d\nu = \int_0^\infty a_\nu\,B_\nu[T(r)]\,d\nu$$

LTE

radiative equilibrim

Auxiliary equations:

$$S_\nu(r) = \varepsilon_\nu(r)\,B_\nu[T(r)]\,[1-\varepsilon_\nu(r)]\,J_\nu(r)$$

$$\varepsilon_\nu(r) \equiv \frac{a_\nu(r)}{a_\nu(r)+\sigma_\nu}$$

Analysis of the sequential procedure

Strong and weak couplings

For the sake of a *classification* of the *different interactions*, we may consider the
range of action of the individual processes

Short range interactions: ***local physics*** ***weak coupling***

Long range interactions : ***transport processes*** ***strong coupling***

From the *algorithmic standpoint*,

The strength measures the *slower or faster flow of information* among the different components of our model

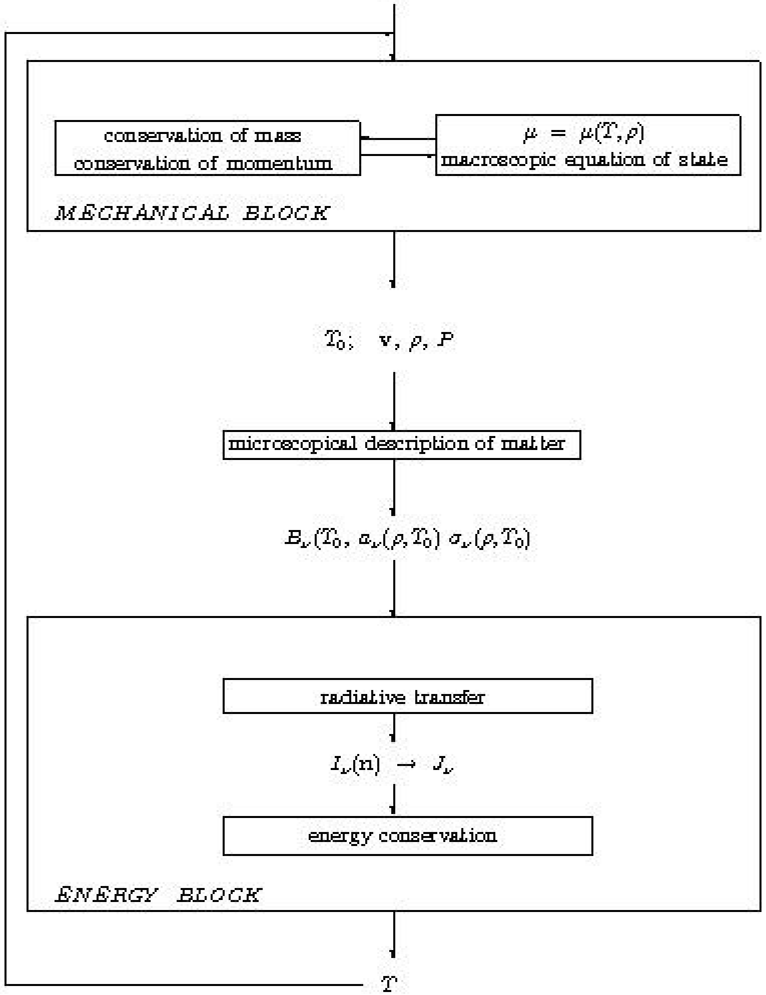
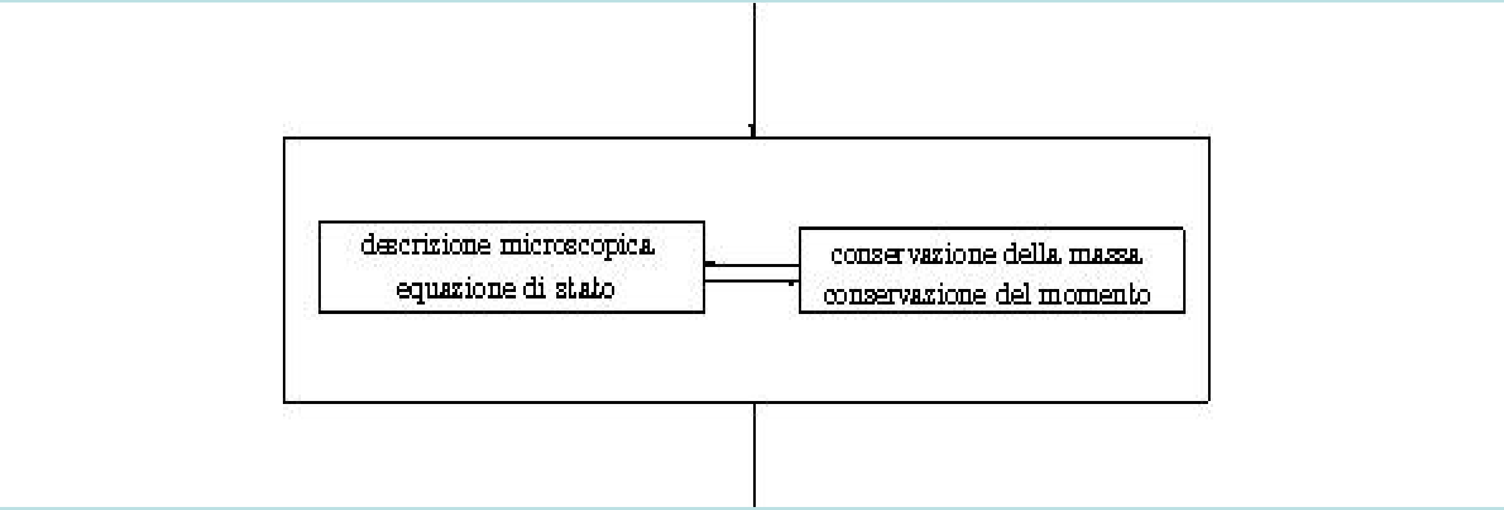


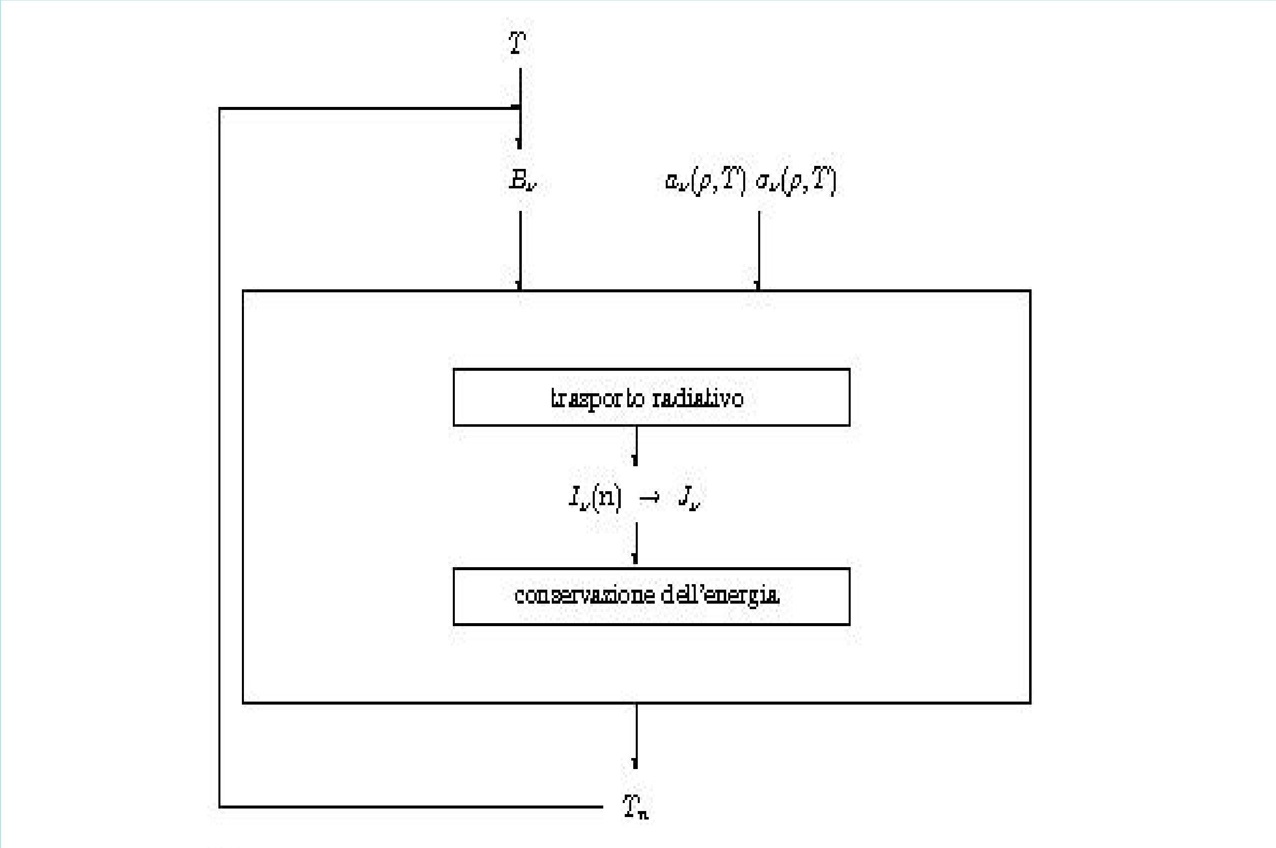
Figure 1: Flow-chart of the natural sequential procedure

The block of the constitutive equations

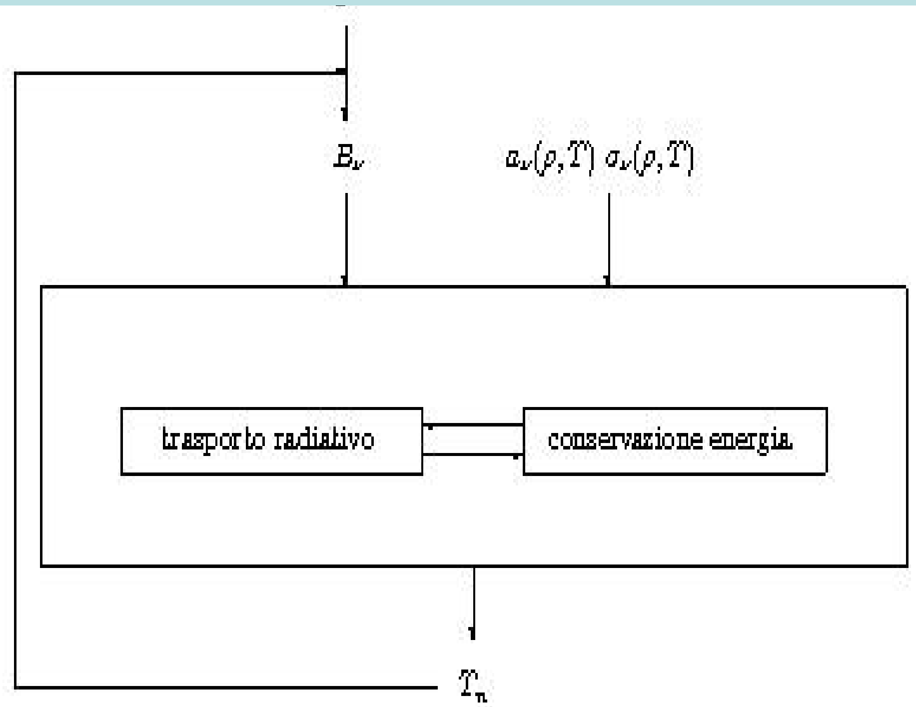


A case of weak coupling

Sequential solution of the energy block. The transport coefficients a_ν and σ_ν are assumed to be data external to the cycle of iterations.



Λ - iteration



The energy block: **simultaneous solution** of the RT and the energy conservation equations. ***Neither this scheme does work.***

The **''hard'' coupling** is brought about by the term

$$J_a \equiv \int_0^\infty a_\nu\, J_\nu\, d\nu$$

The energy block: the simultaneous solution of the RT and the energy conservation equations through the iteration factors.

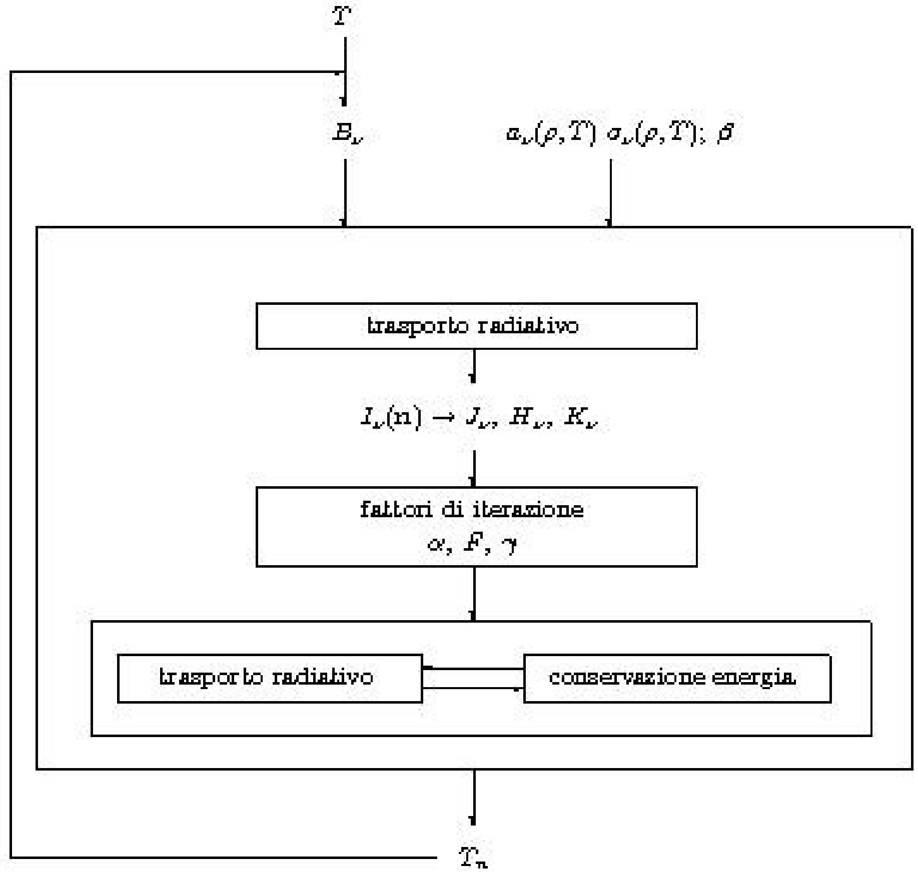


Figura 7: Soluzione iterativa del blocco energetico per mezzo dei fattori di iterazione.

The coupling, through the IFs is now soft !

4. Specific applications and perspectives

The computation of stellar atmosphere model
(as well as models of analogous astrophysical systems)

needs three basic ingredients:

- **The physics**
- **Atomic data**
- **The algorithms**

new problems

(e.g., extended envelopes, winds, magneto hydrodynamics, shocks)

but also, old problems

The old statement by Larry Auer

<< The greatest improvements in the models will not come from the introduction of new physics, but rather by a more adequate treatment of the physics we already know, i.e. non-LTE and line blanketing >>

still hold true thirty years later.

To say nothing of convective transport!

The algorithms (our own future research lines)

- ***The treatment of radiative transfer***

We are facing now the generalization of the Implicit Integral Method in order to compute stellar atmosphere models in spherical geometry.

- ***The self-consistent computation of the structure***

We are going to include the strongest spectral lines into the RE constraint, the necessary step toward a correct estimate of the radiative losses;

as well as the effect of both radiative and convective transport on the temperature distribution with depth.

Basic references:

Some iterative methods for radiative transfer problems

E. Simonneau and L. Crivellari, 2002,
in *Radiative Transfer and Hydrodynamics in Astrophycs,* ESA Publ. Series, Vol. 5.

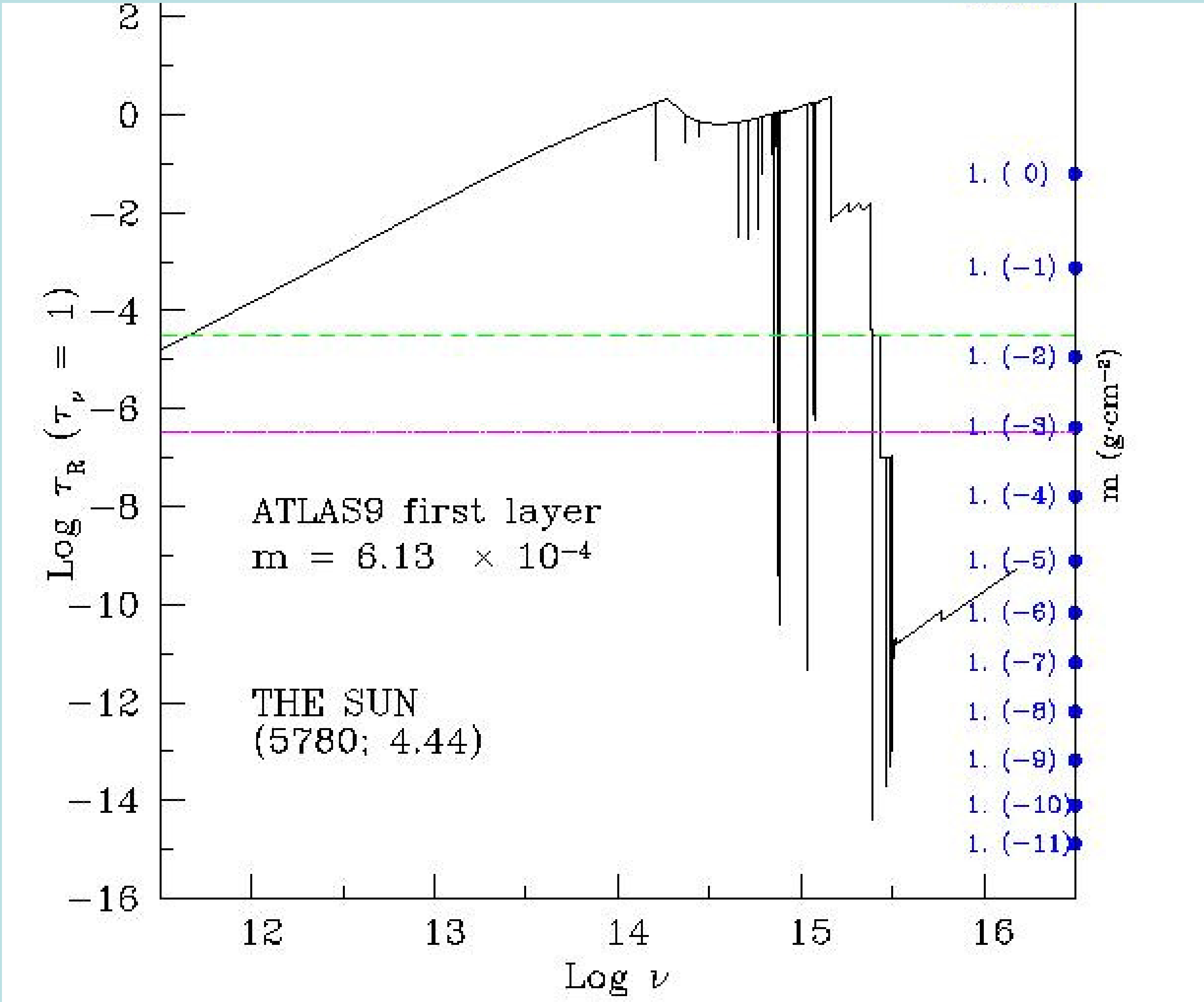
An Implicit Integral Method to solve RT problems in stellar atmospheres

L. Crivellari, 2004, PhD Thesis, (La Laguna: Instituto de Astrofísica de Canarias).

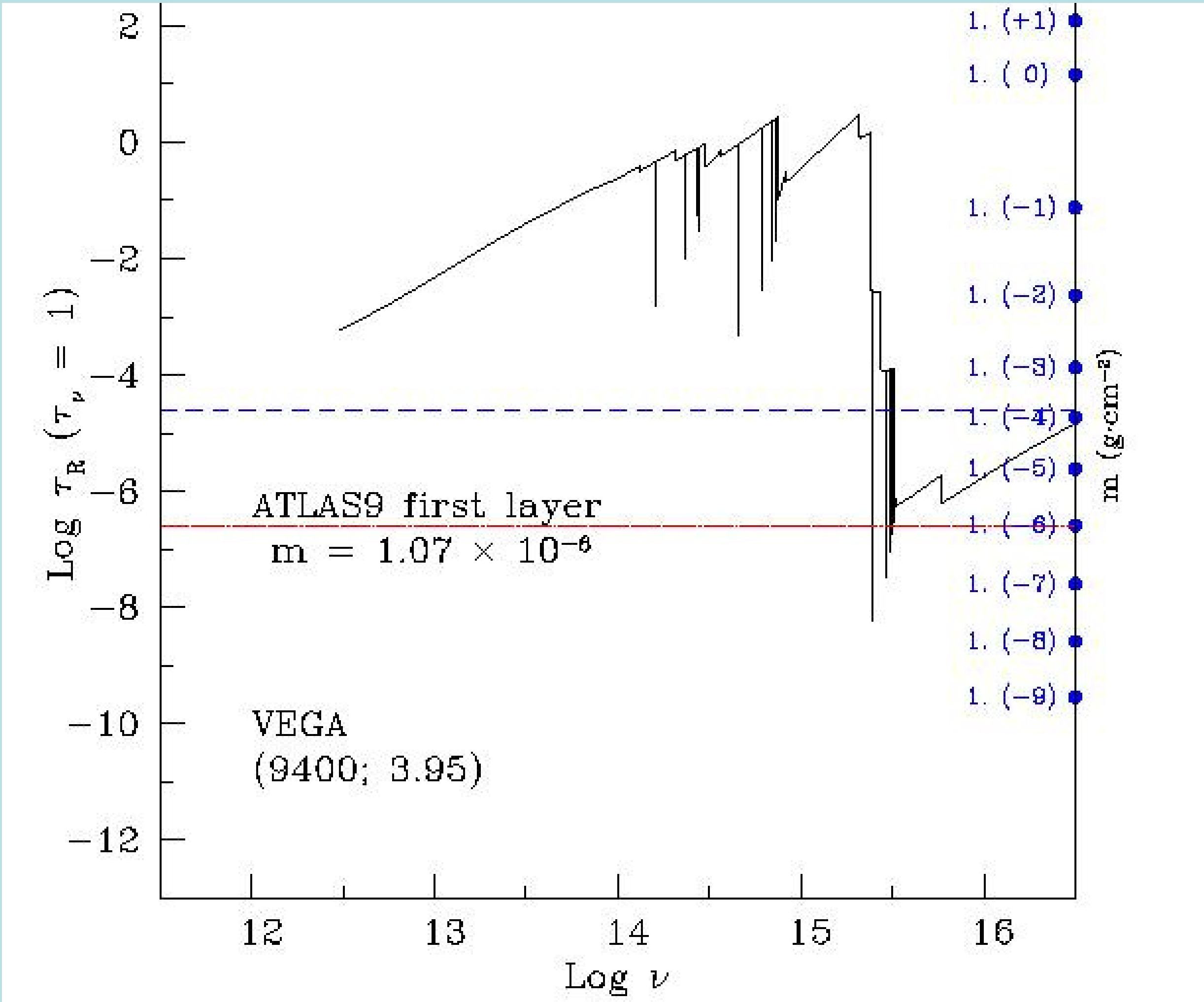
Algorithmic representation of astrophysical structures

L. Crivellari, 2005, in *The Role of Mathematics in Physical Sciences*,
G. Boniolo, P. Budinich and M. Trobok eds, (Dordrecht: Springer), p. 97.

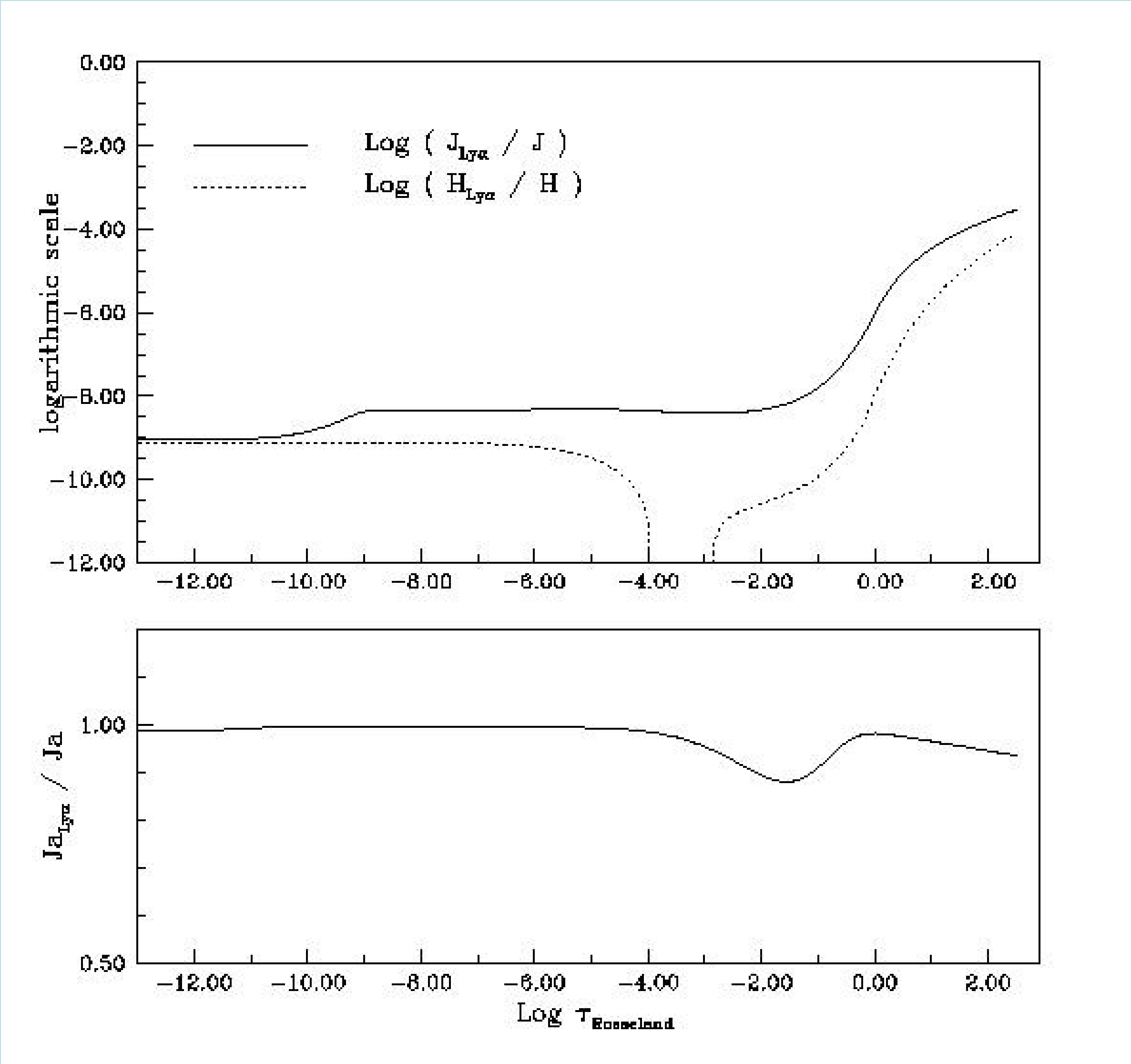
Finis coronat opus



ATLAS9 first layer
m = 6.13 × 10^-4
THE SUN
(5780; 4.44)
Log τ_R (τ_ν = 1)
Log ν
m (g·cm^-2)
1. (0)
1. (−1)
1. (−2)
1. (−3)
1. (−4)
1. (−5)
1. (−6)
1. (−7)
1. (−8)
1. (−9)
1. (−10)
1. (−11)



ATLAS9 first layer
m = 1.07 × 10⁻⁶
VEGA
(9400; 3.95)
Log τ_R (τ_ν = 1)
Log ν
m (g·cm⁻²)
1. (+1)
1. (0)
1. (−1)
1. (−2)
1. (−3)
1. (−4)
1. (−5)
1. (−6)
1. (−7)
1. (−8)
1. (−9)


Log ($J_{Ly\alpha}$ / J)
Log ($H_{Ly\alpha}$ / H)
logarithmic scale
0.00
−2.00
−4.00
−6.00
−8.00
−10.00
−12.00
−12.00 −10.00 −8.00 −6.00 −4.00 −2.00 0.00 2.00
$Ja_{Ly\alpha}$ / Ja
1.00
0.50
Log $\tau_{Rosseland}$

The method of the Iteration Factors

(Simonneau & Crivellari, 1988, *ApJ*, 330,415)

The monochromatic RT equation

$$\mu \frac{dI_\nu(r;\mu)}{dr} = -\chi_\nu(r)\left[I_\nu(r;\mu) - S_\nu(r)\right]$$

$$S_\nu(r) = \varepsilon_\nu(r)\,B_\nu[T(r)] + [1-\varepsilon_\nu(r)]\,J_\nu(r)$$

$$\varepsilon_\nu(r) \equiv \frac{a_\nu(r)}{a_\nu(r)+\sigma_\nu(r)} = \frac{a_\nu(r)}{\chi_\nu(r)}$$

$$J_\nu(r) \equiv \frac{1}{2}\int_{-1}^{1} I_\nu(r;\mu)\,d\mu \;; \qquad H_\nu(r) \equiv \frac{1}{2}\int_{-1}^{1} I_\nu(r;\mu)\,\mu\,d\mu \;; \qquad K_\nu(r) \equiv \frac{1}{2}\int_{-1}^{1} I_\nu(r;\mu)\,\mu^2\,d\mu$$

$$\frac{dH_\nu(r)}{dr} = -\chi_\nu(r)\left[J_\nu(r) - S_\nu(r)\right] = -a_\nu(r)\left[J_\nu(r) - B_\nu(r)\right]$$

$$\frac{dK_\nu(r)}{dr} = -\chi_\nu(r)\,H_\nu(r)$$

$$\frac{1}{\chi_R(r)} \equiv \frac{\int_0^\infty \frac{1}{\chi_R(r)}\frac{\partial}{\partial T} B_\nu[T(r)]\,d\nu}{\int_0^\infty \frac{\partial}{\partial T} B_\nu[T(r)]\,d\nu}$$

monochromatic

$$\chi_H(r) \equiv \frac{\int_0^\infty \chi_\nu(r)\,H_\nu(r)\,d\nu}{\int_0^\infty H_\nu(r)\,d\nu} = \frac{\int_0^\infty \chi_\nu(r)\,H_\nu(r)\,d\nu}{H(r)}$$

The fundamental equations of the stellar atmosphere problem

eq. meccaniche

$$\frac{\partial}{\partial t}\rho + \nabla\cdot(\rho \mathbf{v}) = 0$$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla\cdot(\rho \mathbf{v}\mathbf{v}) = \rho \mathbf{g} - \nabla P$$

eq. di stato

$$P = \frac{k}{m_H \mu}\rho T$$

eq. energetiche

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho v^2 + \mathcal{U}(T)\right] + \nabla\cdot\left[\frac{1}{2}\rho v^2 + \mathcal{U}(T)\right]\mathbf{v} = \rho \mathbf{v}\cdot\mathbf{g} + \nabla(P\mathbf{v})$$

$$\frac{\partial}{\partial t}u + \nabla\cdot\mathcal{F} = \int d\nu \oint d\Omega\,(\eta_\nu - \chi_\nu I_\nu)$$

eq. del trasporto radiativo

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \mathbf{n}\cdot\nabla\right) I_\nu = \eta_\nu - \chi_\nu I_\nu$$

descrizione dello stato microscopico

$$\mu,\ \eta_\nu,\ \chi_\nu$$

$$ETL : f(\rho,T)\ ; \qquad non - ETL : f(\rho,T;[J_\nu])$$

Def.: $$\beta(\tau) \equiv \frac{\chi_H(\tau)}{\chi_H(\tau)}$$

we obtain the new equation: $$\frac{d}{d\tau} F(\tau)\, J(\tau) = \beta(\tau)\, H \quad ,$$

$$\gamma \equiv \frac{J(\tau=0)}{H}$$

with the initial condition: $$J(\tau=0) = \gamma\, H$$

whose trivial solution is

$$J(\tau) = \frac{H}{F(\tau)} \left[\gamma\, F(\tau=0) + \int_{\tau=0}^{\tau} \beta(t)\, d\,t \right]$$

Temperature correction

Def.

$$a_P \equiv \frac{\int_0^\infty a_\nu \, B_\nu(T) \, d\nu}{\int_0^\infty B_\nu(T) \, d\nu}$$

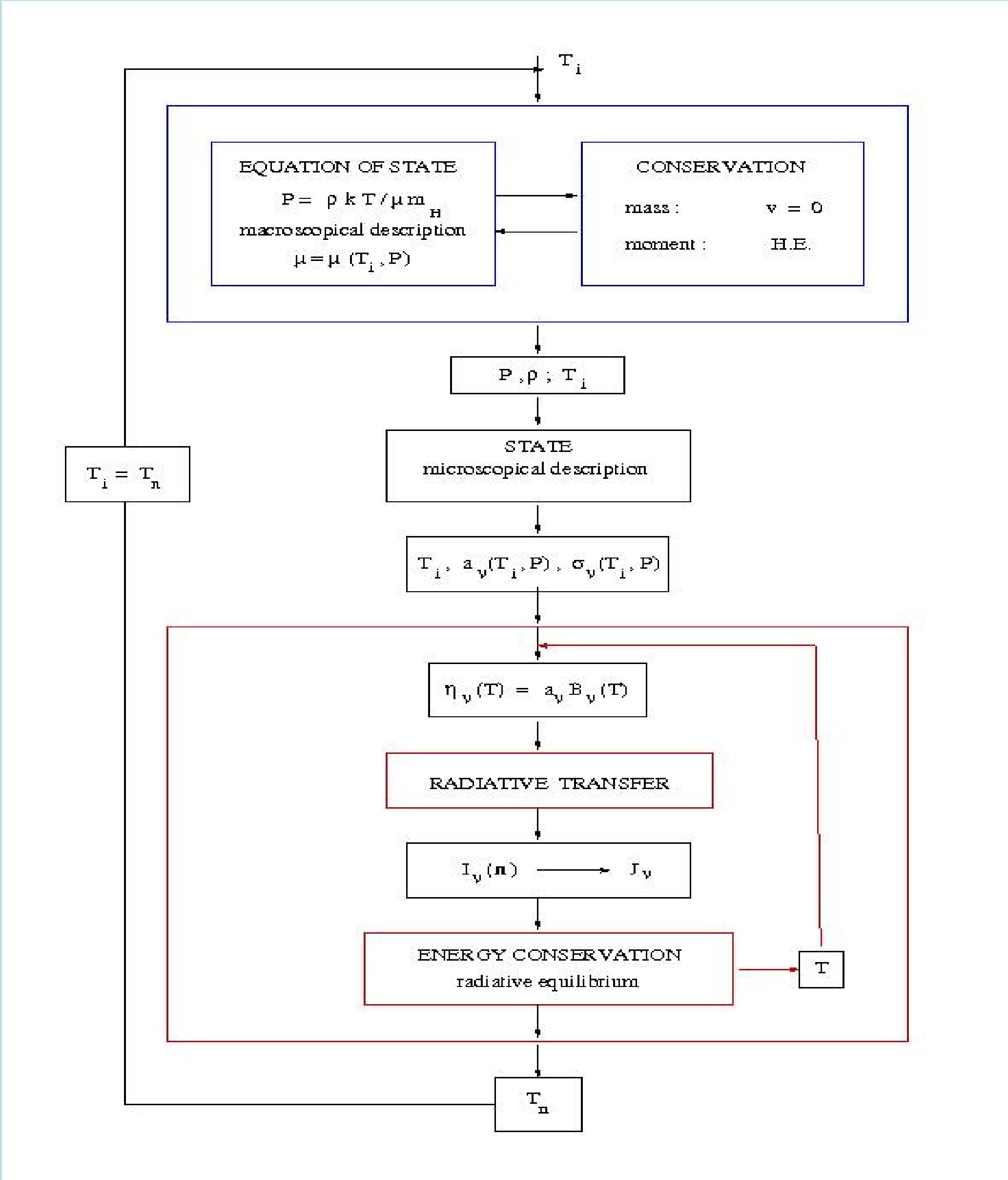
$$a_J \equiv \frac{\int_0^\infty a_\nu \, J_\nu \, d\nu}{\int_0^\infty J_\nu \, d\nu}$$

$$\alpha(\tau) \equiv \frac{a_J(\tau)}{a_P(\tau)}$$

The constraint of radiative equilibrium impose:

$$a_P B = a_J J \longrightarrow B[T(\tau)] = \alpha(\tau) \, J(\tau)$$

$$T(\tau) = \sqrt[4]{\frac{\sigma}{\pi} \alpha(\tau) \, J(\tau)}$$


T i
EQUATION OF STATE
P = ρ k T / μ m H
macroscopical description
μ = μ (T i , P)
CONSERVATION
mass : v = 0
moment : H.E.
P , ρ ; T i
STATE
microscopical description
T i = T n
T i , a ν(T i , P) , σ ν(T i , P)
η ν (T) = a ν B ν (T)
RADIATIVE TRANSFER
I ν (n) J ν
ENERGY CONSERVATION
radiative equilibrium
T
T n

<< The whole system, for all depths and frequencies, can be organized into a form suitable for a Rybicki-method solution. Thus let

$$\boldsymbol{\delta}\mathbf{J}_n \equiv \left(\delta J_{1n}, \delta J_{2n}, \ \dots \ \delta J_{Dn}\right)^T, \quad (n = 1, \dots, N)$$

$$\boldsymbol{\delta}\mathbf{T} \equiv \left(\delta T_1, \delta T_2, \ \dots \ \delta T_D\right)^T$$

$$\boldsymbol{\delta}\mathbf{N} \equiv \left(\delta N_1, \delta N_2, \ \dots \ \delta N_D\right)^T$$

Then equations (7-39), (7-52) *and* (7-53) *yield*

$$\begin{pmatrix} \mathbf{T}_1 & 0 & \dots & 0 & \mathbf{U}_1 & \mathbf{V}_1 \\ 0 & \mathbf{T}_2 & & & \mathbf{U}_2 & \mathbf{V}_2 \\ . & & & & . & . \\ . & & & & . & . \\ . & & & 0 & . & . \\ 0 & & \dots & \mathbf{T}_N & \mathbf{U}_N & \mathbf{V}_N \\ \mathbf{W}_1 & \mathbf{W}_2 & \dots & \mathbf{W}_N & \mathbf{A} & \mathbf{B} \\ \mathbf{X}_1 & \mathbf{X}_2 & \dots & \mathbf{X}_N & \mathbf{C} & \mathbf{D} \end{pmatrix} \begin{pmatrix} \boldsymbol{\delta}\mathbf{J}_1 \\ \boldsymbol{\delta}\mathbf{J}_2 \\ \\ \\ \\ \boldsymbol{\delta}\mathbf{J}_N \\ \boldsymbol{\delta}\mathbf{N} \\ \boldsymbol{\delta}\mathbf{T} \end{pmatrix} = \begin{pmatrix} \mathbf{K}_1 \\ \mathbf{K}_2 \\ \\ \\ \\ \mathbf{K}_N \\ \mathbf{L} \\ \mathbf{M} \end{pmatrix} \qquad (7-57)$$

Each element in equation (7-57) is a matrix of dimension $(D \times D)$ *>>*

(*From Mihalas, Stellar Atmospheres (1978), p. 184*)

$$\int_0^\infty a_\nu \; J_\nu \; d\nu \;=\; \int_0^\infty a_\nu \; B(T)_\nu \; d\nu$$

RE equation

Linearization of the Planck function

$$B_\nu(T) \;=\; B_\nu(T_0) \;+\; \left(\frac{\partial B_\nu}{\partial T}\right)_{T_0} (T - T_0)$$

$$J_a \;=\; \int_0^\infty a_\nu \; B_\nu(T_0)\, d\nu \;+\; (T - T_0) \int_0^\infty a_\nu \left(\frac{\partial B_\nu}{\partial T}\right)_0 d\nu$$

$$T - T_0 \;=\; \frac{J_a \;-\; \int_0^\infty a_\nu \; B_\nu(T_0)\, d\nu}{\int_0^\infty a_\nu \left(\frac{\partial B_\nu}{\partial T}\right)_0 d\nu}$$

$$B_\nu(T) \;=\; f_1(\nu;T_0) \;+\; f_2(\nu;T_0)\, J_a$$

$$S_\nu \;=\; \varepsilon_\nu \; \left[f_1(\nu;T_0) + f_\nu(\nu;T_0)\, J_a \right] \;+\; (1 - \varepsilon_\nu)\, J_\nu$$

The source function including the RE constraint

change of variable: $d\tau \equiv -\chi_R(r)\, dr$

$$\frac{d\,H_\nu(r)}{d\,\tau} = -\frac{a_\nu(r)}{\chi_R(\tau)}\left[J_\nu(\tau) - B_\nu(\tau)\right]$$

$$\frac{d\,K_\nu(r)}{d\,\tau} = -\frac{\chi_\nu(r)}{\chi_R(\tau)} H_\nu(\tau)$$

$$\frac{d\,H(r)}{d\,\tau} = -\frac{1}{\chi_R(\tau)}\left[\int_0^\infty a_\nu J_\nu(\tau)\, a_\nu J_\nu(\tau)\, d\nu - \int_0^\infty a_\nu J_\nu(\tau)\, a_\nu J_\nu(\tau)\, d\nu\right] = 0$$

$$\frac{d\,K(r)}{d\,\tau} = -\frac{\chi_H(r)}{\chi_R(\tau)} H(\tau)$$

bolometric

$$H(\tau) = H = \frac{\sigma_R}{4\pi} T_{eff}^4$$

$$\frac{d\,K(\tau)}{d\,\tau} = \frac{\chi_H(\tau)}{\chi_H(\tau)} H$$

$$\frac{K(\tau)}{J(\tau)} = F(\tau)$$

new relation: approximate closure