The ionization, excitation and thermal state of flows in the ISM

A. Raga (Instituto de Ciencias Nucleares, UNAM)

1. Gasdynamic equations (3D, Cartesian)

continuity equation →

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} \rho u_j = 0 \,, \tag{1}$$

momentum equation (3 components) →

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j + P \delta_{ij}) = 0 \,, \tag{2}$$

energy equation →

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} [u_j (E + P)] = G - L \,, \tag{3}$$

with $E = \rho u_j u_j / 2 + P/(\gamma - 1)$ (γ is the specific heat ratio, $= 5/3$ for our discussion of a non-relativistic, atomic/ionic gas).

Heading and cooling: contributions from many species

$$G = \sum_{a} G_a \, ; \quad L = \sum_{a} L_a \, , \tag{4}$$

Continuity equations for all of the species:

$$\frac{\partial n_a}{\partial t} + \frac{\partial}{\partial x_j} n_a u_j = S_a \,, \tag{5}$$

Alternative, transport form:

$$\frac{\partial y_a}{\partial t} + u_j \frac{\partial}{\partial x_j} y_a = \frac{S_a}{n} \,, \tag{6}$$

where $y_a = n_a/n$ is the fractional abundance of the species a (with $n = \rho/m$, m being the average mass per atom or ion).

Rate equations for a constant density gas

$$\frac{dn_{a,z}}{dt} = S^{c}{}_{a,z} + S^{ph}{}_{a,z} \,, \tag{7}$$

with the collisional (S^{c}) and photoionisation (S^{ph}) source terms being given by

$$S^{c}{}_{a,z} = n_e \left[n_{a,z-1} c_{a,z-1} + n_{a,z+1} \alpha_{a,z+1} - n_{a,z} \left(c_{a,z} + \alpha_{a,z} \right) \right] \,, \tag{8}$$

$$S^{ph}{}_{a,z} = n_{a,z-1} \phi_{a,z-1} - n_{a,z} \phi_{a,z} \,. \tag{9}$$

The electron density

$$n_e = \sum_a \sum_z z \, n_{a,z} \,. \tag{10}$$

→ Charge exchange reactions

Collisional ionisation and radiative+dielectronic recombination coefficients:

$$\alpha(T),\ c(T) = \int_0^\infty f(v,T)\sigma_v\, v\, dv\,, \tag{11}$$

Arrhenius:

It is common to give analytic fits to these coefficients in the "Arrhenius interpolation" form :

$$r(T) = b_1\, T^{b_2}\, e^{b_3/T}\,. \tag{12}$$

Aldrovandi & Pequignot (1973, 1976)

$$r(T) = b_1 \left(\frac{T}{10^4}\right)^{-b_2} + b_3 T^{-3/2} \exp\left(-b_4/T\right) \left[1 + b_5 \exp\left(-b_6/T\right)\right]\,, \tag{13}$$

for recombination coefficients.

Table 1: Ionisation, recombination and charge exchange coefficients

reaction	coefficients[a]
e + HI → 2e + HII	1: 5.83×10^{-11}, 0.5, -157800
e + HII → HI	1: 3.69×10^{-10}, -0.79, 0
e + HeI → 2e + HeII	1: 2.707×10^{-11}, 0.5, -285400
e + HeII → HeI	2: 4.3×10^{-13}, 0.672, 0.0019, 4.7×10^{5}, 0.3, 94000
e + HeII → 2e + HeIII	1: 5.711×10^{-12}, 0.5, -631000
e + HeIII → HeII	1: 2.21×10^{-9}, -0.79, 0
e + CII → 2e + CIII	1: 3.93×10^{-11}, 0.5. -283000
e + CIII → CII	2: 3.2×10^{-12}, 0.770, 0.038, 9.1×10^{4}, 2.0, 3.7×10^{5}
e + CIII → 2e + CIV	1: 2.04×10^{-11}, 0.5, -555600
e + CIV → CIII	2: 2.3×10^{-12}, 0.645, 7.03×10^{-3}, 1.5×10^{5}, 0.5, 2.3×10^{5}
e + NI → 2e + NII	1: 6.18×10^{-11}, 0.5 -168200
e + NII → NI	2: 1.5×10^{-12}, 0.693, 0.0031 2.9×10^{5}, 0.6, 1.7×10^{5}
e + NII → 2e + NIII	1: 4.21×10^{-11}, 0.5, -343360
e + NIII → NII	2: 4.4×10^{-12}, 0.675, 0.0075 2.6×10^{5}, 0.7, 4.5×10^{5}
e + OI → 2e + OII	1: 1.054×10^{-10}, 0.5, -157800
e + OII → OI	2: 2.0×10^{-12}, 0.646, 0.0014 1.7×10^{5}, 3.3, 5.8×10^{4}
e + OII → 2e + OIII	1: 3.53×10^{-11}, 0.5, -407200
e + OIII → OII	2: 3.1×10^{-13}, 0.678, 0.0014 1.7×10^{5}, 2.5, 1.3×10^{5}
e + OIII → 2e + OIV	1: 1.656×10^{-11}, 0.5, -636900
e + OIV → OIII	2: 5.1×10^{-12}, 0.666, 0.0028 1.8×10^{5}, 6.0, 91000
e + SII → 2e + SIII	1: 7.12×10^{-11}, 0.5, -271440
e + SIII → SII	2: 1.8×10^{-12}, 0.686, 0.0049 1.2×10^{5}, 2.5, 88000
HI + NII → HII + NI	1: 1.1×10^{-12}, 0, 0
HII + NI → HI + NII	1: 4.95×10^{-12}, 0. -10440
HI + OII → HII + OI	1: 2.0×10^{-9}, 0, 0
HII + OI → HI + OII	1: 1.778×10^{-9}, 0, -220

[a] The interpolation formulae are of the form "1:" Arrhenius, or "2:" Aldrovandi & Péquignot (1973), see equations (12) and (13)

Photoionization rates:

$$\phi_{a,z} = \int_{\nu_{a,z}}^{\infty} \frac{4\pi J_\nu}{h\nu} \sigma_{a,z}(\nu)\, d\nu \,, \tag{14}$$

Radiative transfer equation:

$$\frac{dI_\nu}{dl} = j_\nu - \kappa_\nu I_\nu \tag{15}$$

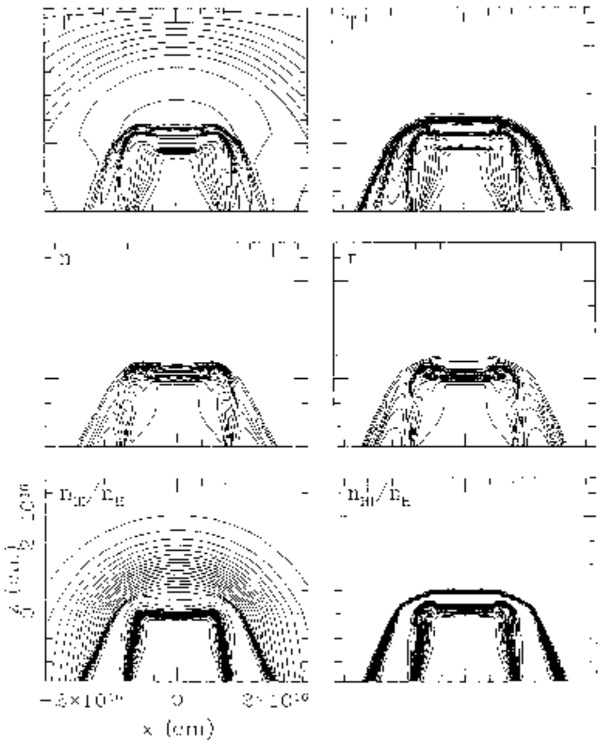
Average intensity:

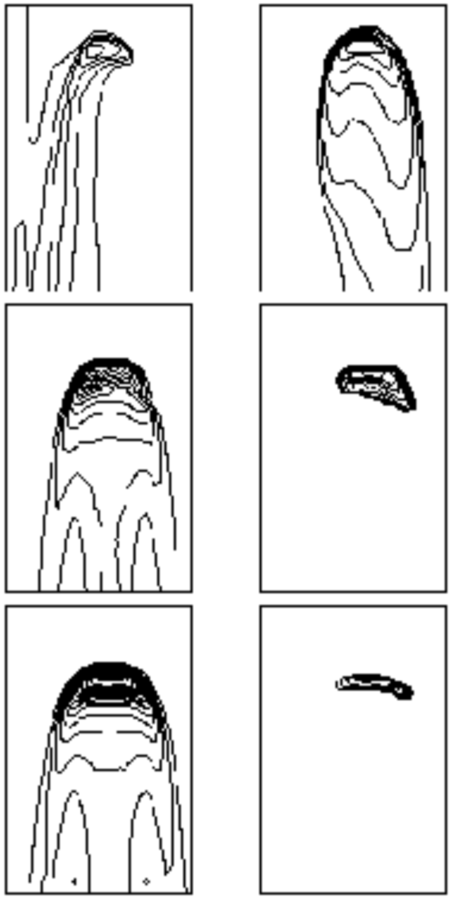
$$J_\nu = \frac{1}{4\pi} \oint I_\nu d\Omega \tag{16}$$

→Included in 1D (stationary and time-dependent) shock models

→Two papers in which the “diffuse” ionisation field is included

→Of order 20 papers in which an external ionising field is included (flows in HII regions)





Standard calculations:

→ S and C are assumed to be at least singly ionised

→ Photoionisation (and associated heating) neglected

Coronal ionisation equilibrium (S=0):

$$n_{a,z} C_{a,z} = n_{a,z+1} \alpha_{a,z+1} \,. \tag{17}$$

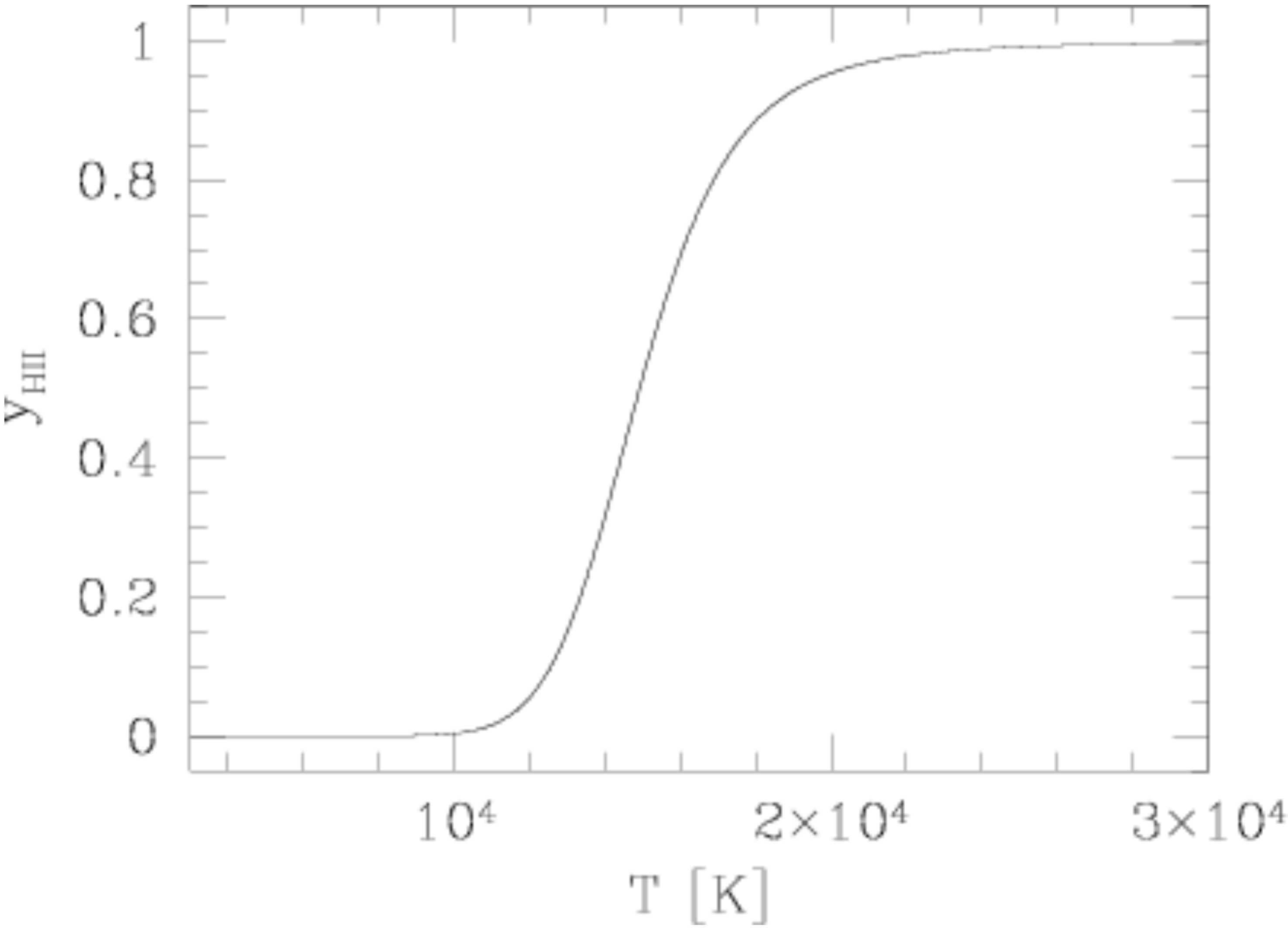
Equilibrium for H:

$$n_{HI} c(T) = n_{HII} \alpha(T) \,. \tag{18}$$

We can combine this equation with $n_H = n_{HI} + n_{HII}$ to obtain

$$y_{HII} = \frac{n_{HII}}{n_H} = \frac{1}{1 + \alpha(T)/c(T)} \,, \tag{19}$$

where the Arrhenius interpolations for the coefficients are $\alpha(T) = 3.69 \times 10^{-10} T^{-0.79}$ and $c(T) = 5.83 \times 10^{-11} T^{0.5} e^{-157800/T}$


1
0.8
0.6
0.4
0.2
0
y_{HII}
10^4
2×10^4
3×10^4
T [K]

The cooling function:

Recombination and free-free cooling:

$$L_{ff}(HII) = n_e n_{HII} \beta_{ff}(T)\,, \tag{20}$$

where the interpolation formula

$$\beta_{ff}(z,T) = 1.846 \times 10^{-27} z^2 T^{1/2}\,, \tag{21}$$

$$L_{rec}(HII) = n_e n_{HII} \beta_{rec}(T)\,, \tag{22}$$

where the interpolation formula

$$\beta_{rec}(t) = 1.133 \times 10^{-24} t^{-1/2} \left(-0.0713 + 0.5 \ln t + 0.640 t^{-1/3}\right) \tag{23}$$

with $t = 157890/T$ (see Seaton 1959).

$$\beta_{rec}(z,T) = z\beta_{rec}(1, T/z^2)\,, \tag{24}$$

Collisional ionisation:

$$L^{ion}{}_{a,z} = n_e n_{a,z} c_{a,z}(T)\, \chi_{a,z}\,, \qquad (25)$$

Collisionally excited lines:

l=1,…N : excited levels

$$n_{a,z} = \sum_{l=1}^{N} n_l \, . \tag{26}$$

Energy loss→

$$L_{a,z}^{\mathrm{col}} = \sum_{l=1}^{N} n_l \sum_{m<l} A_{l,m} h\nu_{l,m} \, , \tag{27}$$

Populations of the excited levels→

$$\sum_{m>l} n_m A_{m,l} + n_e \sum_{m \neq l} n_m q_{m,l}(T) = n_l \left[\sum_{m<l} A_{m,l} + n_e \sum_{m \neq l} q_{l,m}(T) \right] , \qquad (28)$$

$$n_{a,z} = \sum_{l=1}^{N} n_l \, . \qquad (26)$$

→Linear system of equations for the populations of the N levels

Collisional de-excitation coefficient→

$$q_{m,l}(T) = \frac{8.629\times 10^{-6}}{T^{1/2}}\frac{\Omega_{ml}(T)}{g_m}\,, \tag{29}$$

Collisional excitation coefficient→

$$q_{l,m}(T) = \frac{g_m}{g_l}e^{-h\nu_{m,l}/kT}q_{m,l}(T)\,. \tag{30}$$

Collision strengths → Chianti database

A coefficients

The 3-level atom:

$$n_1 + n_2 + n_3 = n_{a,z}\,. \tag{31}$$

Now, for $l = 1$, from equation (28) we obtain

$$n_1\left[-n_e(q_{12} + q_{13})\right] + n_2(A_{21} + n_e q_{21}) + n_3(A_{31} + n_e q_{31}) = 0\,, \tag{32}$$

and for $l = 2$, we obtain :

$$n_1(n_e q_{12}) + n_2\left[-A_{21} - n_e(q_{23} + q_{21})\right] + n_3(A_{32} + n_e q_{32}) = 0\,. \tag{33}$$

→ System of 3 linear equations

2-level atom:

Equation (26) takes the form

$$n_{a,z} = n_1 + n_2 \, , \tag{34}$$

and equation (28) takes the form

$$n_1 n_e q_{12} = n_2 (n_e q_{21} + A_{21}) \, . \tag{35}$$

Solution→

$$n_2 = \frac{n_{a,z}}{(g_1/g_2) e^{E_{21}/kT} + 1 + n_c/n_e} \, , \tag{36}$$

where the critical density is defined as $n_c \equiv A_{21}/q_{12}$.

Low and high density regimes:

for $n_e \ll n_c$ (the "low density regime"), we have

$$n_2 = \frac{n_{a,z} n_e q_{12}}{A_{21}} \, , \tag{37}$$

and for $n_e \gg n_c$ (the "high density regime"), we have

$$n_2 = \frac{n_{a,z} g_2 e^{-E_{21}/kT}}{g_1 + g_2 e^{-E_{21}/kT}} \, , \tag{38}$$

Cooling: general, low and high density regime

$$L_{21} = n_2 A_{21} h\nu_{21} \, , \tag{39}$$

which for the low density regime then takes the form

$$L_{21} = n_{a,z} n_e q_{12} h\nu_{21} \, , \tag{40}$$

and for the high density regime becomes

$$L_{21} = n_2(LTE) A_{21} h\nu_{21} \, , \tag{41}$$

Recipes for calculating the cooling function

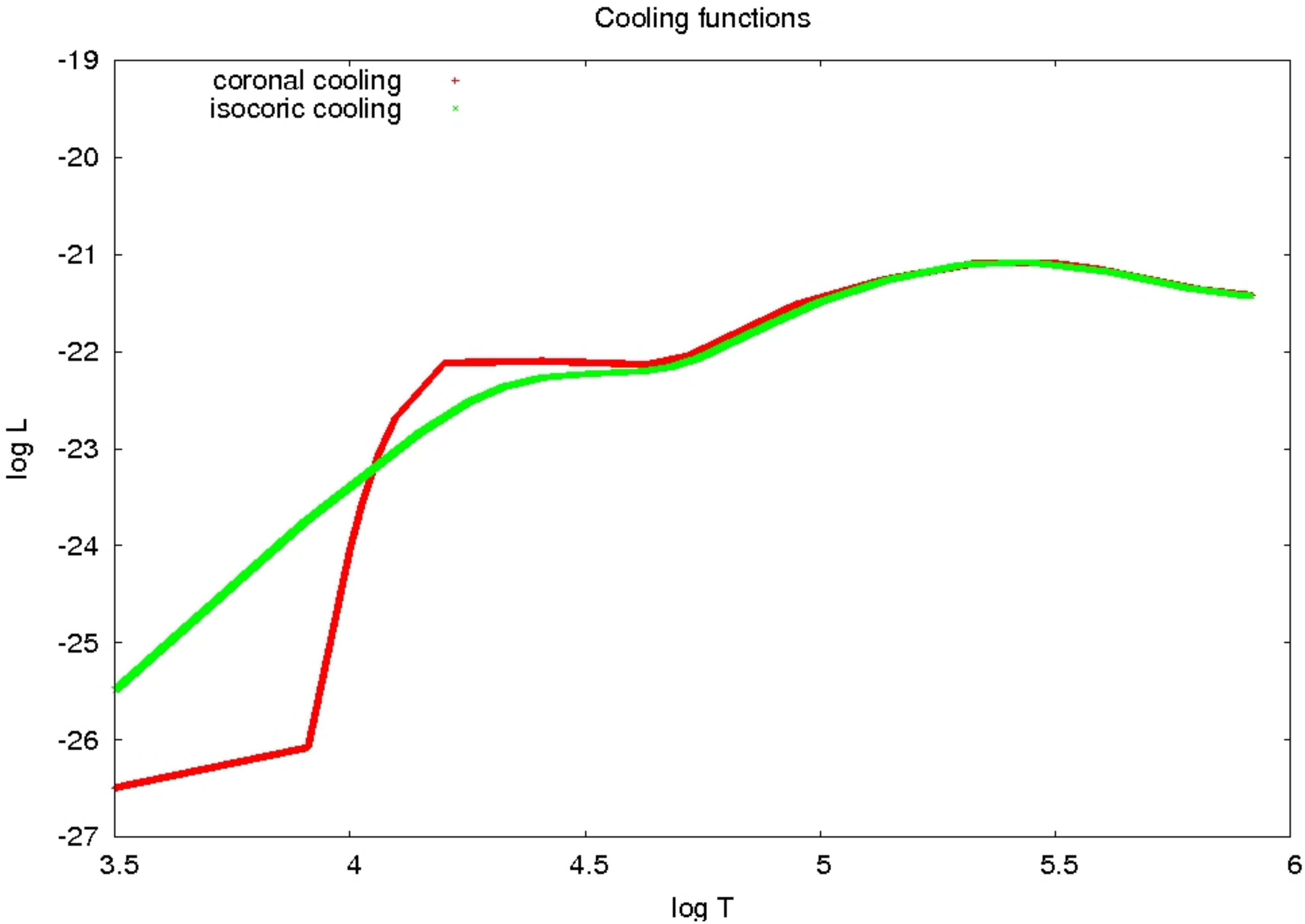
2 most simple approaches:

→Coronal ionisation cooling function

→Isochoric cooling function

$$\frac{3}{2}\frac{d}{dt}(n+n_e)kT=-L\,, \tag{42}$$

Both tabulated as a function of T (for n=1)


Cooling functions
coronal cooling
isocoric cooling
log L
log T
-19
-20
-21
-22
-23
-24
-25
-26
-27
3.5
4
4.5
5
5.5
6

→Tabulations of cooling functions for many ions

(as a function of n and T)

→Fits to the low density regime cooling (as a function of T, for n=1)

$$\log_{10}\left(\frac{L_{OI}}{n_e n_{OI}}\right) = -45.0 + 1.23t_1 + 0,5{t_1}^{10} + 1.2t_2 + 1.2\left[\max(t_2,0)\right]^{7}, \quad (43)$$

$$\log_{10}\left(\frac{L_{OII}}{n_e n_{OI}}\right) = -47.3 + 7.9t_3 + 1.9\frac{t_4}{|t_4|^{0.5}}\,, \quad (44)$$

with $t_1 = 1 - 100/T$, $t_2 = 1 - 10^4/T$, $t_3 = 1 - 2000/T$, $t_4 = 1 - 5 \times 10^4/T$.

Single-species non-equilibrium cooling:

→ Single continuity/rate equation for HI (or HII)

→Assume that the OI/II ionisation follows HI/II

→Consider only HI collisional ionisation + OI/OII collisionally excited line cooling

→Has to include a switch to other cooling function above 20000 K

Cooling:

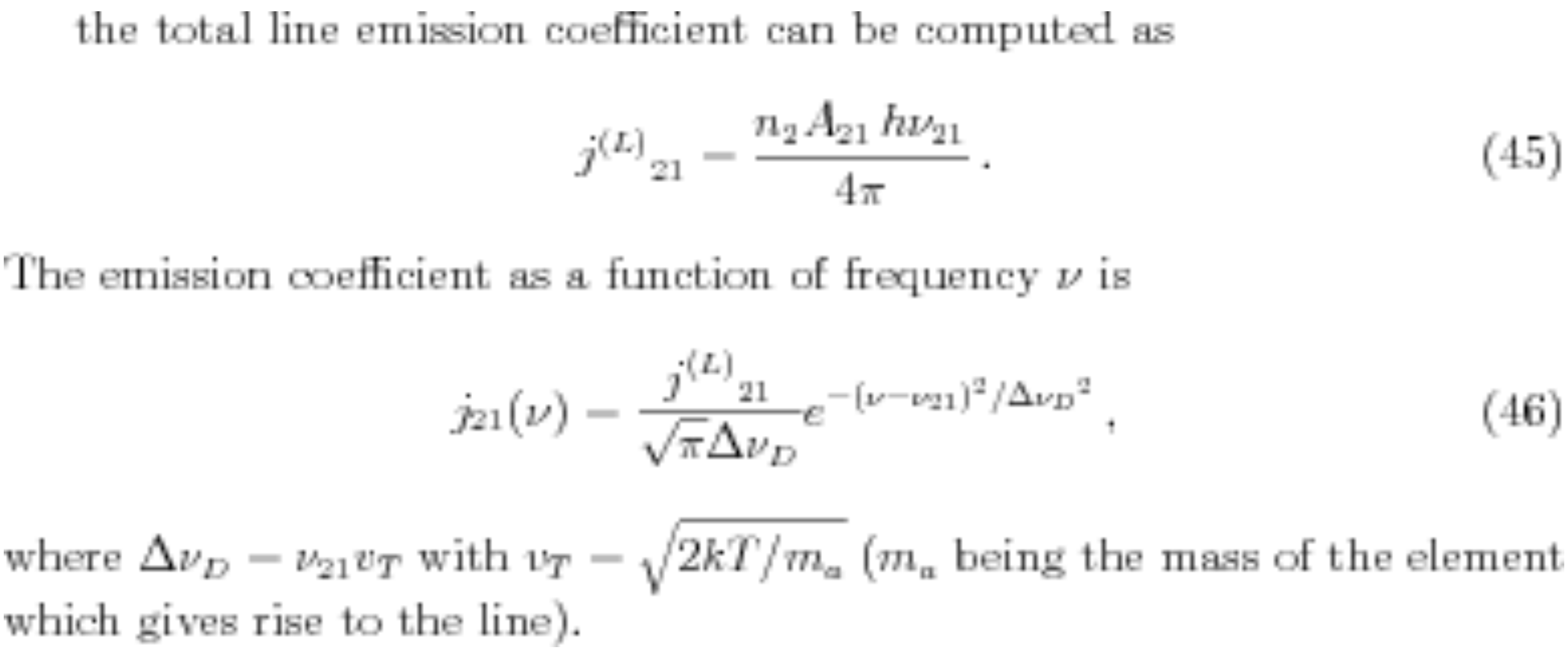
→coronal, isochoric

→single species non-equilibrium

→many species non-equilibrium

Calculation of the emitted spectrum

the emission coefficient→



the total line emission coefficient can be computed as

$$j^{(L)}{}_{21} = \frac{n_2 A_{21}\, h\nu_{21}}{4\pi}\,. \tag{45}$$

The emission coefficient as a function of frequency ν is

$$j_{21}(\nu) = \frac{j^{(L)}{}_{21}}{\sqrt{\pi}\Delta\nu_D} e^{-(\nu-\nu_{21})^2/\Delta\nu_D{}^2}\,, \tag{46}$$

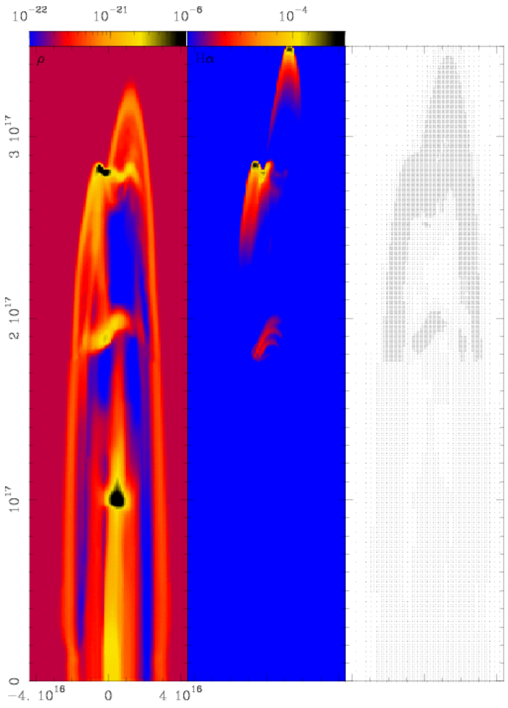
where $\Delta\nu_D = \nu_{21} v_T$ with $v_T = \sqrt{2kT/m_a}$ (m_a being the mass of the element which gives rise to the line).

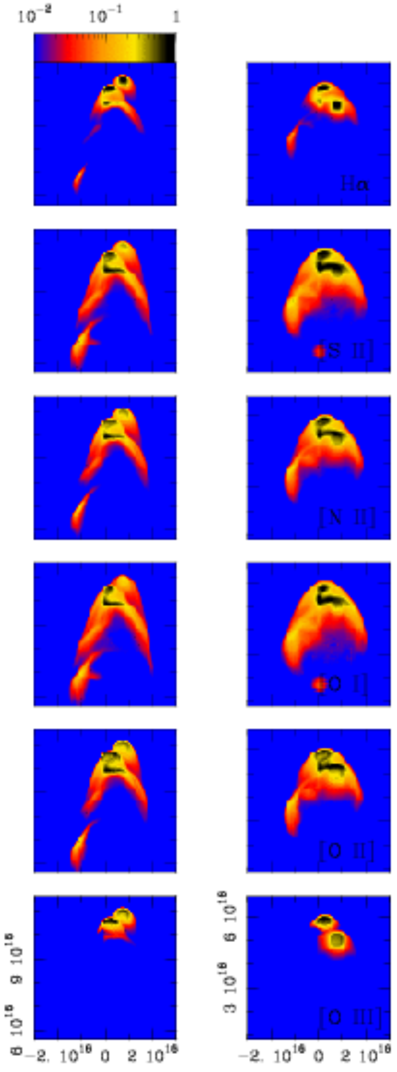
as a function of radial velocity:

$$j_{21}(v_r) = \frac{j^{(L)}{}_{21}}{\sqrt{\pi}v_T} e^{-v_r{}^2/v_T{}^2}\,. \tag{47}$$

predicted emission line intensity map:

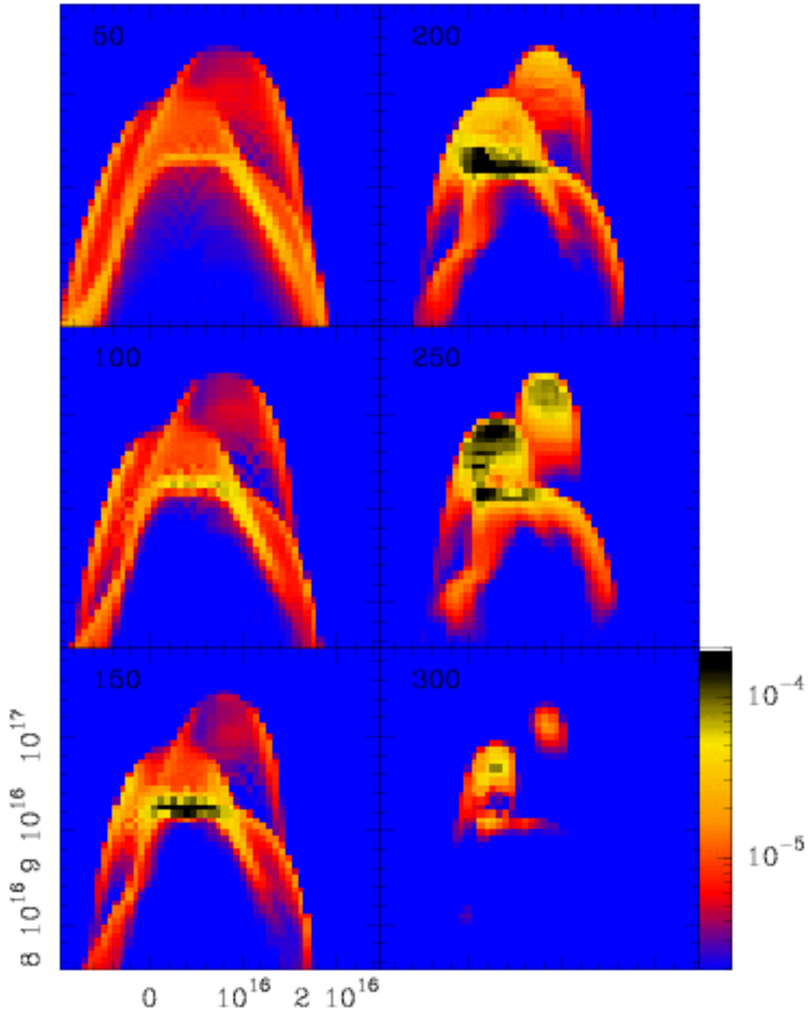
$$I_{21}(x,y) = \int j^{(L)}{}_{21}(x,y,z)\,dz\,,$$

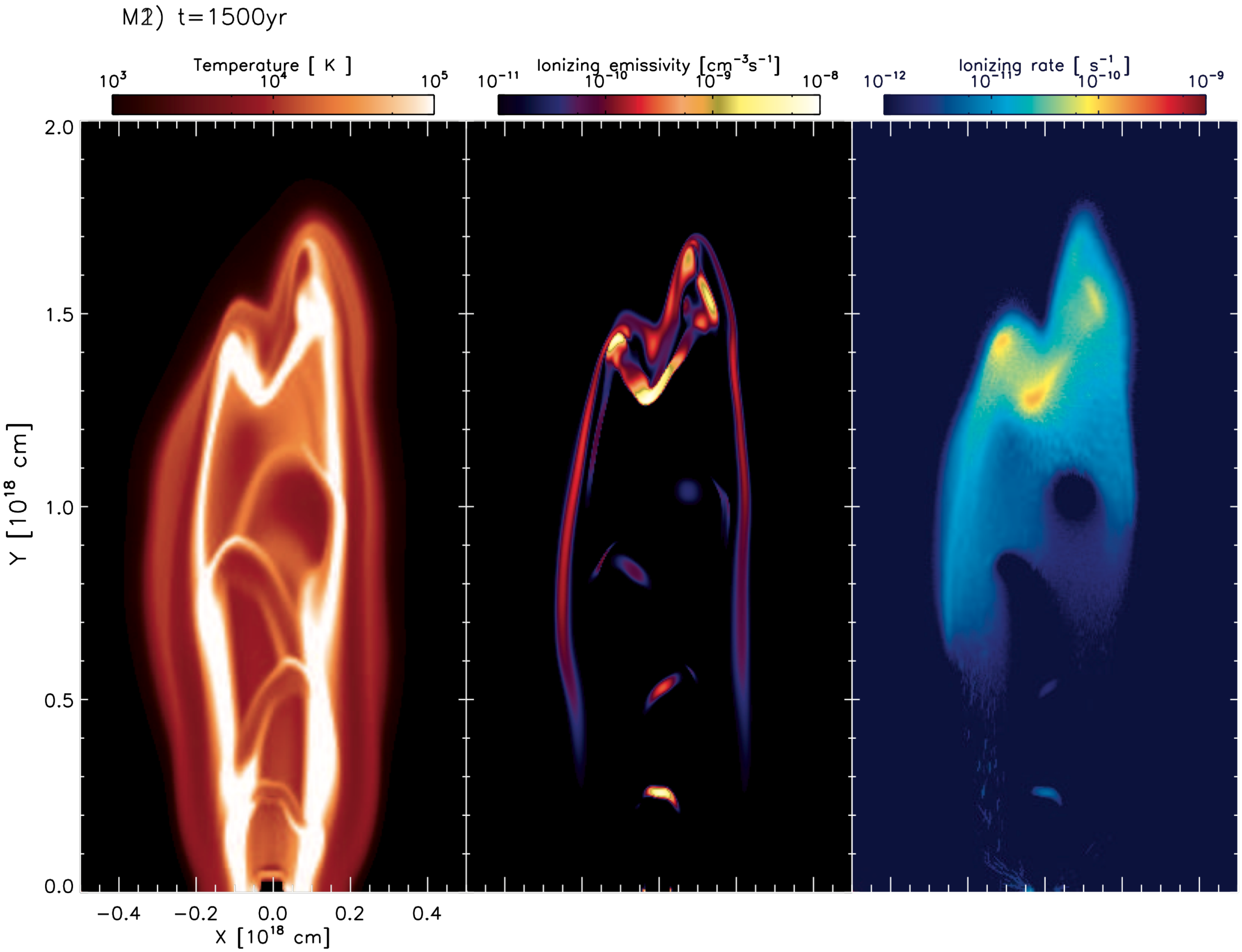


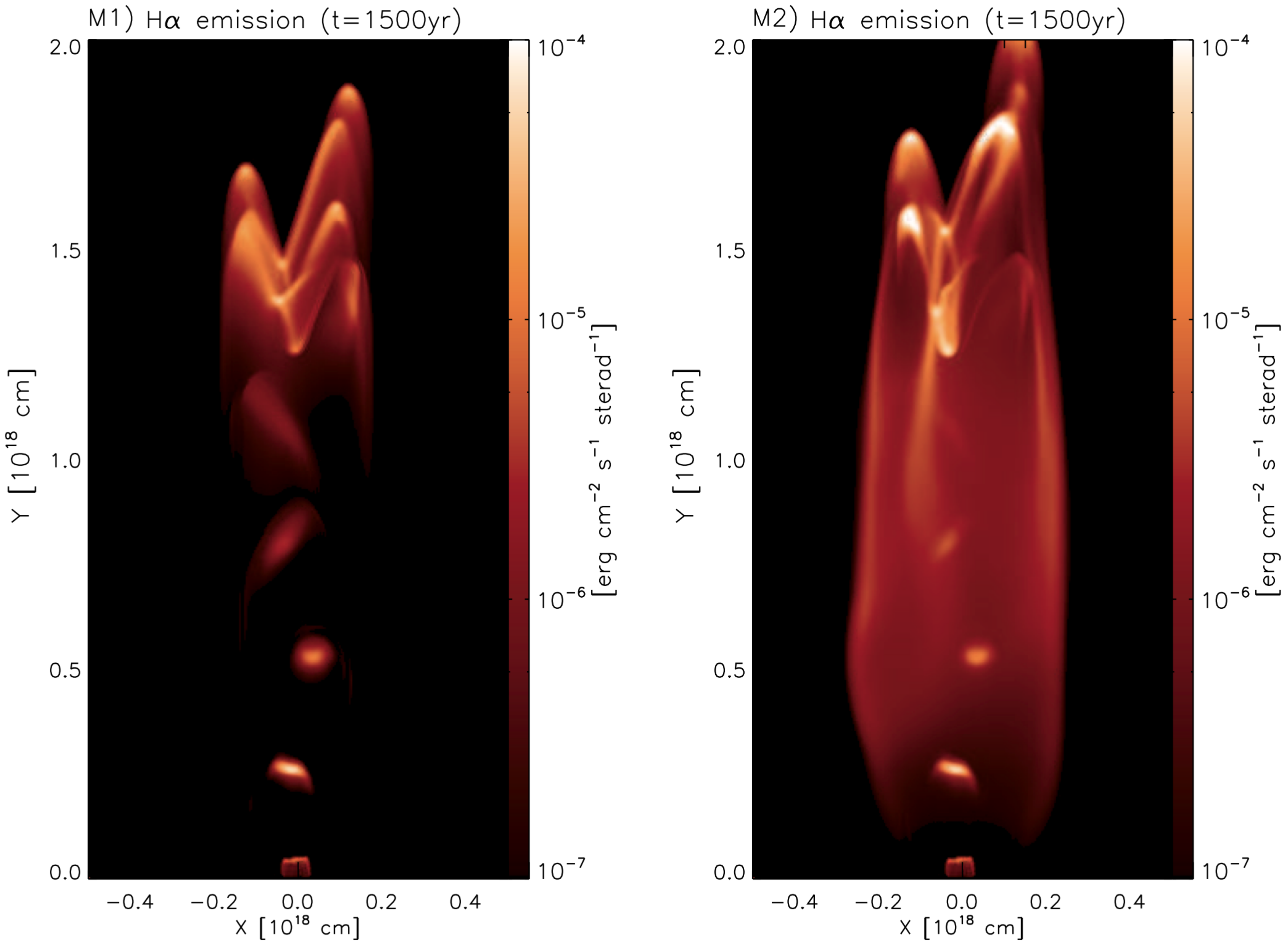


predicted velocity channel maps

$$I_{21}(v_r, x, y) = \int j_{21}(v_r - v^{(f)}{}_r, x, y, z)\, dz\,, \qquad (49)$$




M2) t=1500yr
Temperature [K]
10^3
10^4
10^5
Ionizing emissivity [cm^-3 s^-1]
10^-11
10^-10
10^-9
10^-8
Ionizing rate [s^-1]
10^-12
10^-11
10^-10
10^-9
2.0
1.5
1.0
0.5
0.0
Y [10^18 cm]
−0.4
−0.2
0.0
0.2
0.4
X [10^18 cm]


M1) Hα emission (t=1500yr)
M2) Hα emission (t=1500yr)
Y [10^18 cm]
X [10^18 cm]
2.0
1.5
1.0
0.5
0.0
−0.4
−0.2
0.0
0.2
0.4
10^−4
10^−5
10^−6
10^−7
[erg cm^−2 s^−1 sterad^−1]

Optically thick lines

$$\tau_{21}(v_r, x, y, z) = \int_{-\infty}^{z} \kappa_{21}(v_r - v^{(f)}{}_r, x, y, z')\, dz' \,, \tag{50}$$

where κ_{21} is the absorption coefficient :

$$\kappa_{21}(v_r, x, y, z) = n_2(x, y, z) \left(\frac{g_2}{g_1}\right) \frac{c^2 A_{21}}{8\pi^{3/2} {\nu_{21}}^2 v_T}\, e^{(-v_r/v_T)^2} \,, \tag{51}$$

$$I_{21}(v_r, x, y) = \int j_{21}(v_r - v^{(f)}{}_r, x, y, z) \exp\left[-\tau_{21}(v_r, x, y, z)\right]\, dz \,. \tag{52}$$

Summary:

the calculation of the cooling function and the ionisation state of the gas can be done in 3 different degrees of complexity:

→coronal equilibrium or isochoric

→single species, non-equilibrium

→many species, non-equilibrium