Geometry Independent Radiative Transfer through Gas and Dust using the Monte Carlo method

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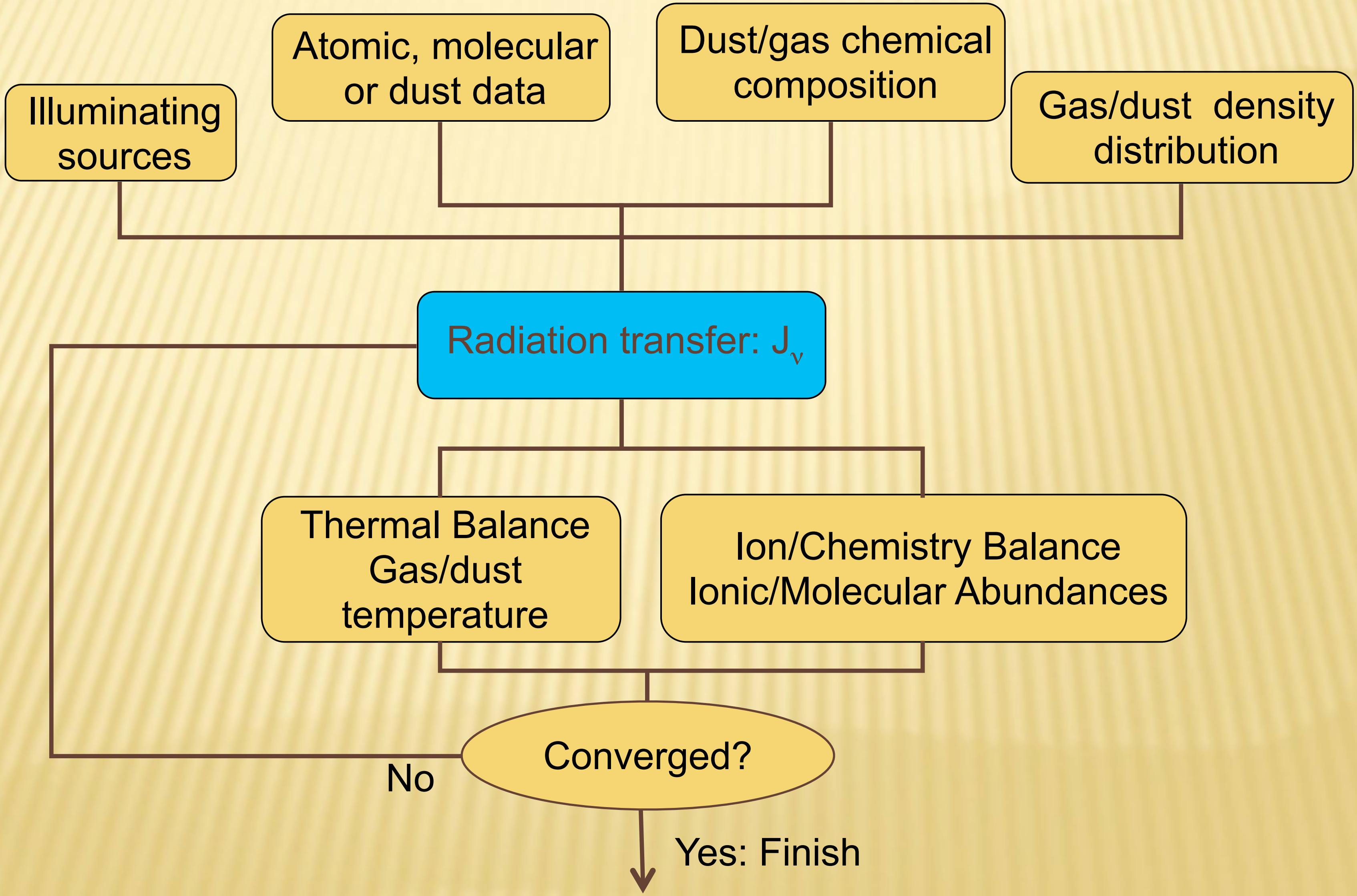
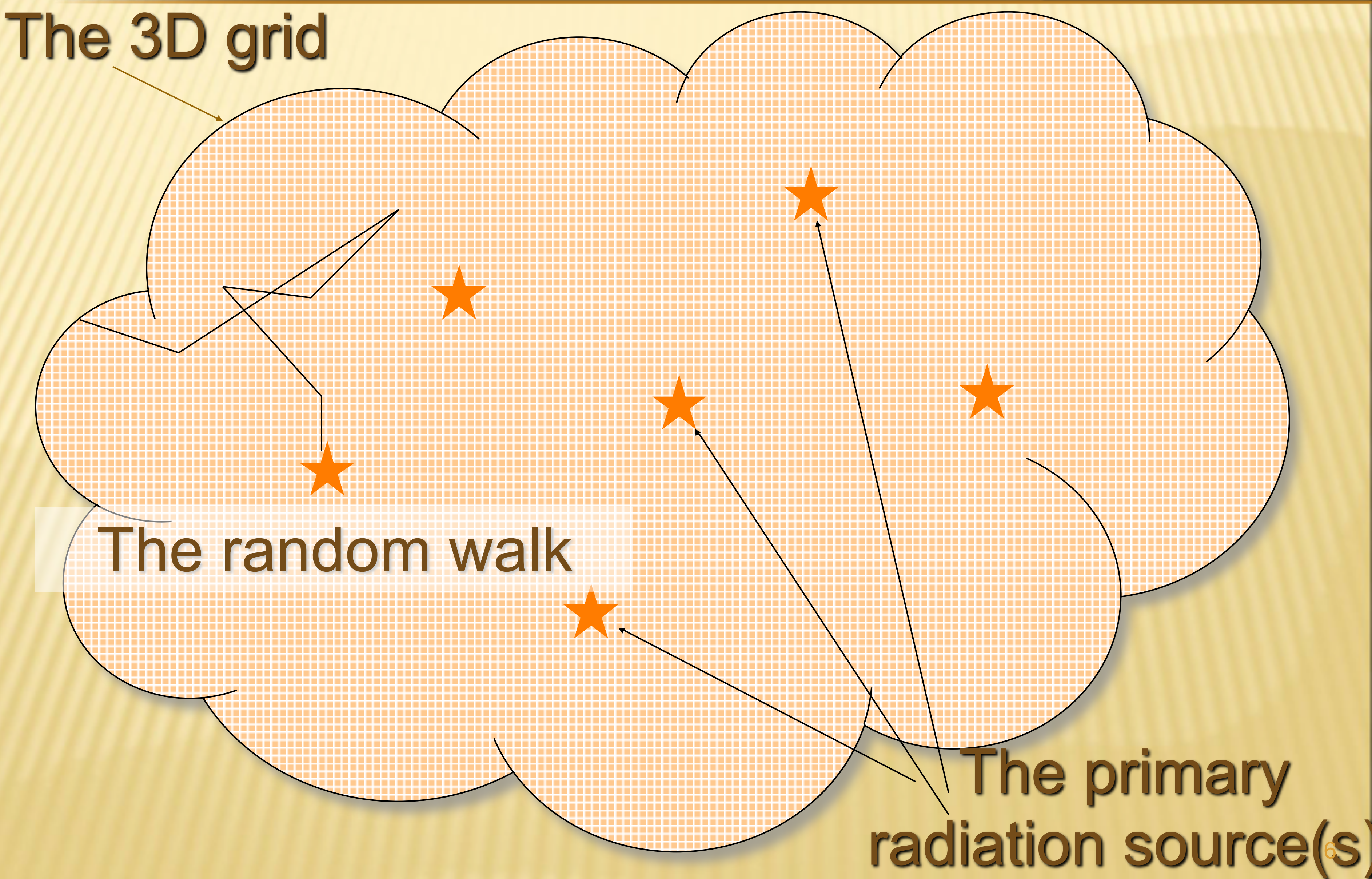
OVERVIEW

- Radiative Transfer Calculations
- Gas & Dust RT with Monte Carlo
- Gas and Dust Thermal Coupling
- The MOCASSIN code
- Questions

RADIATIVE TRANSFER SIMULATIONS

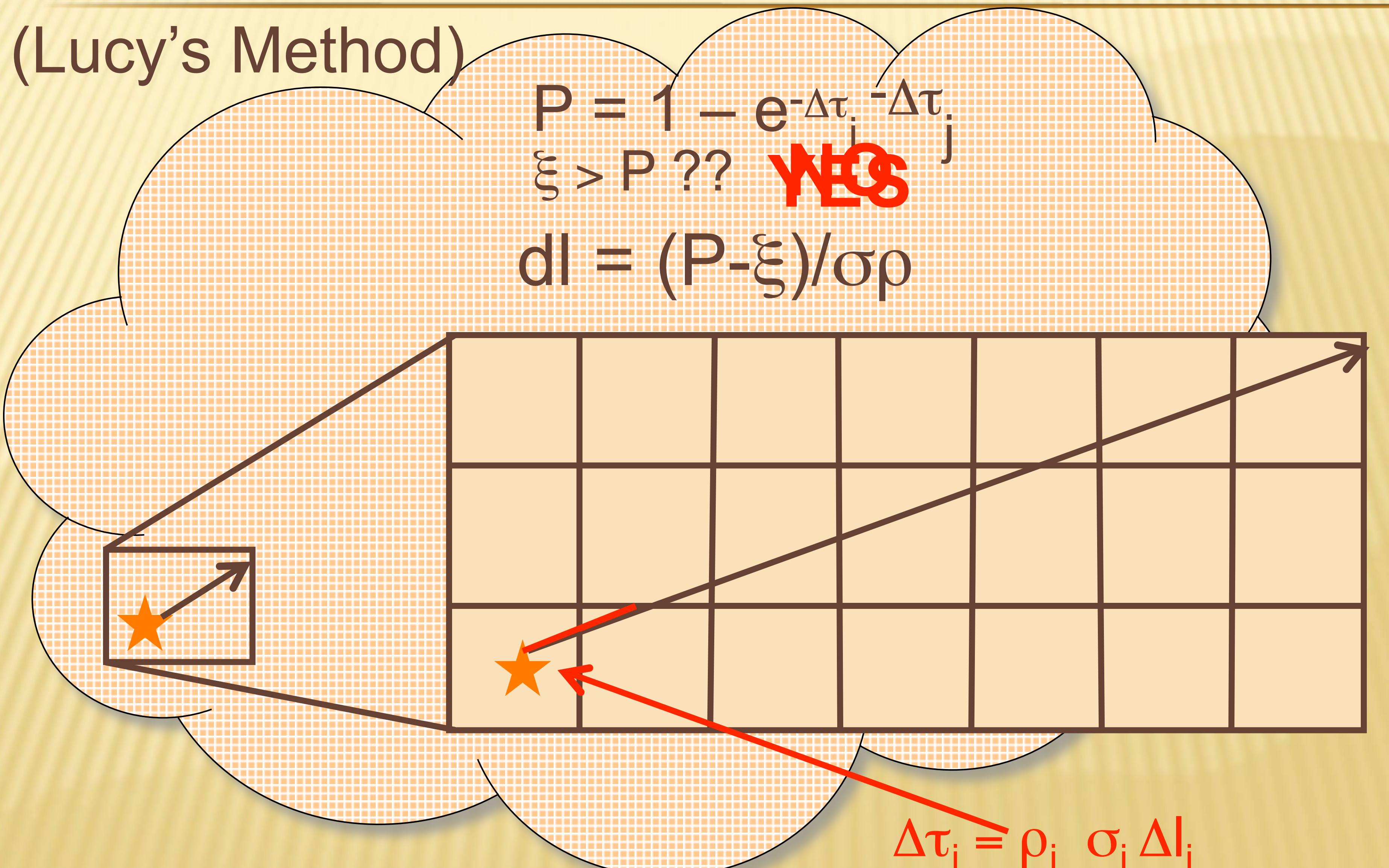


3D MonteCarlo RT: the basics



3D MonteCarlo RT: the basics

(Lucy’s Method)



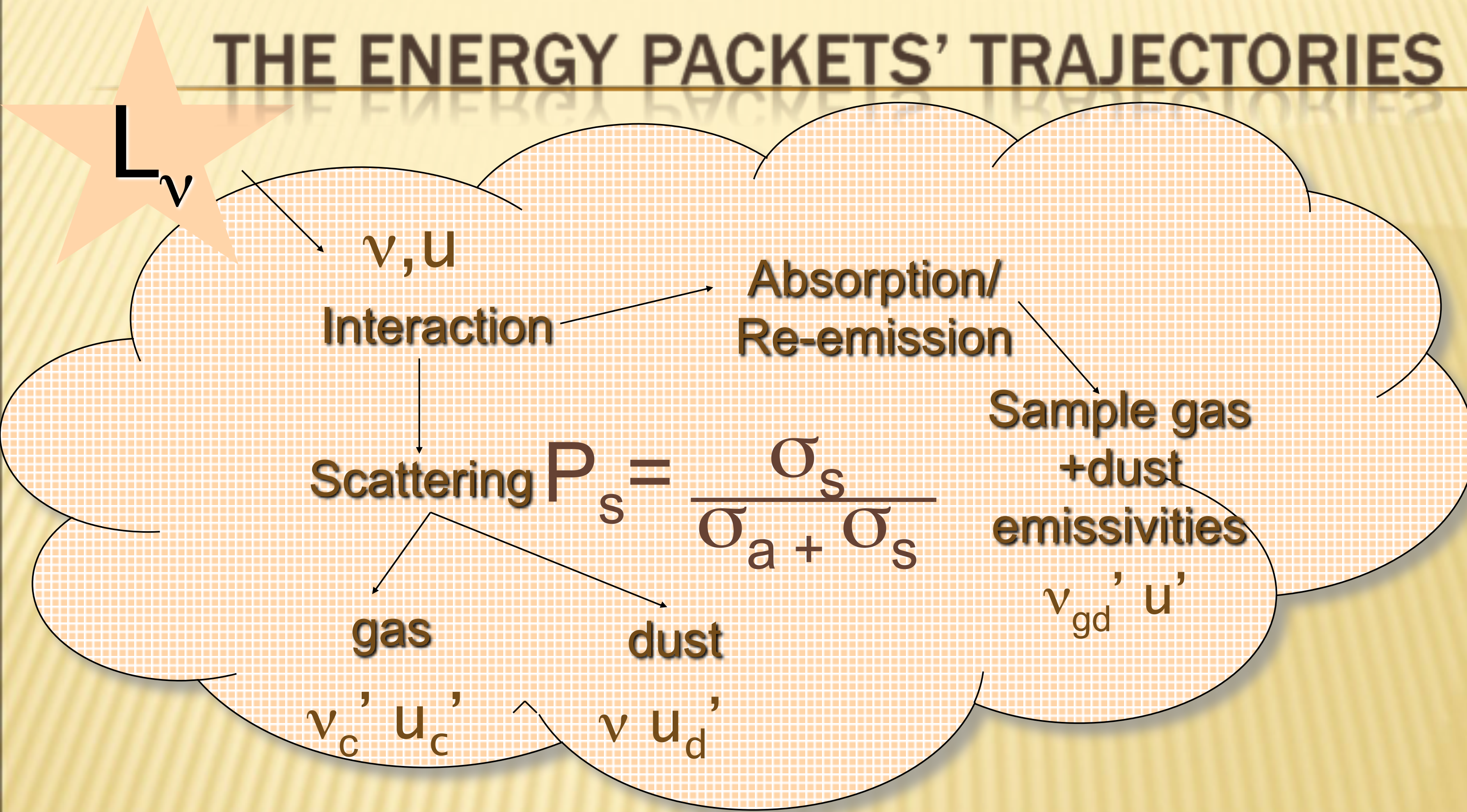
$P = 1 - e^{-\Delta\tau_i}$ $^{-\Delta\tau_j}$

$\xi > P$?? YES NO

$dl = (P - \xi)/\sigma\rho$

$\Delta\tau_i = \rho_i \ \sigma_i \, \Delta l_i$

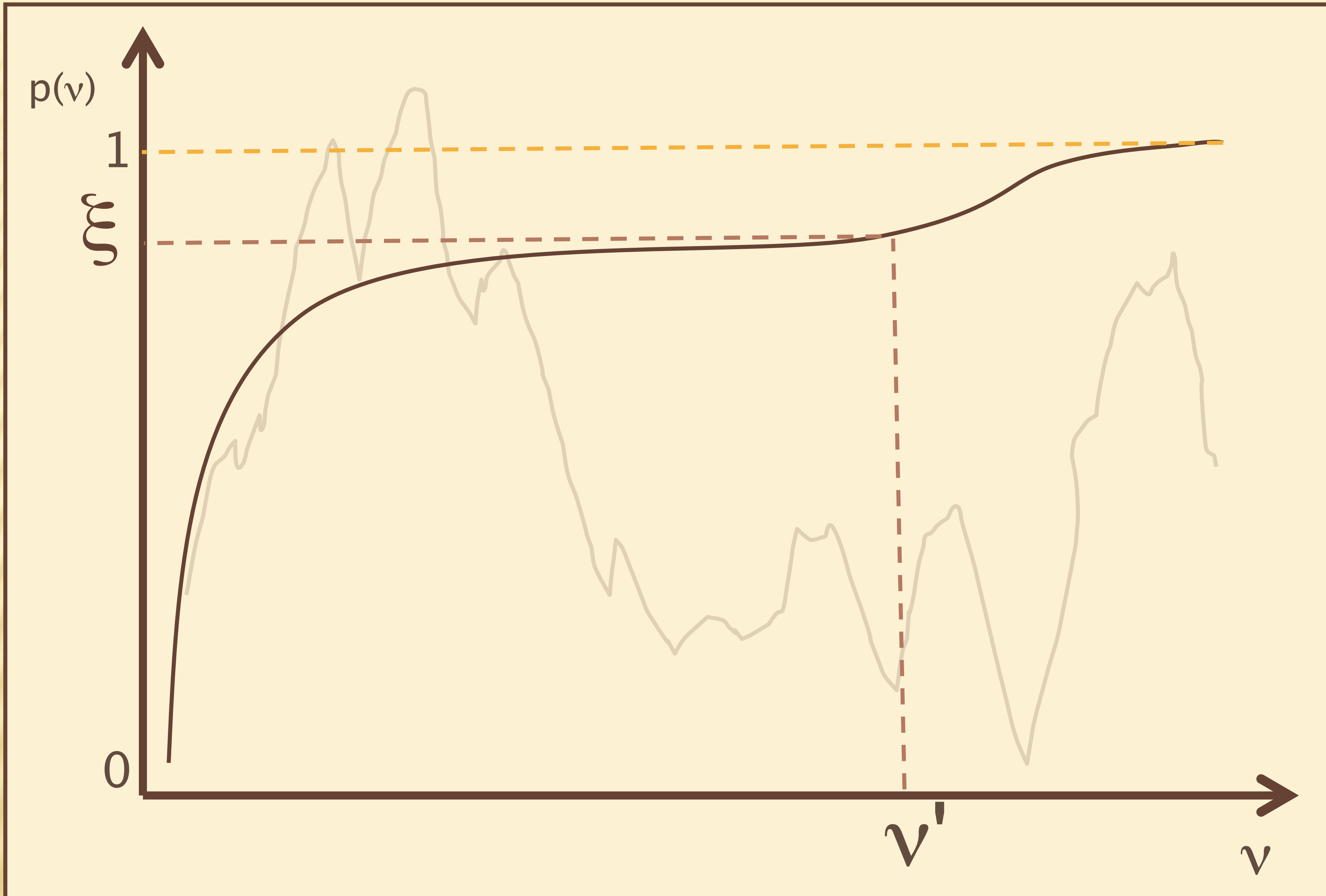
THE ENERGY PACKETS' TRAJECTORIES



u' is chosen at random

u'_c u'_d are chosen according to a phase function

ν'_{gd} is determined by $j_{dust}(\nu)+j_{gas}(\nu)$



$$j_\nu = \qquad p(\nu) = \int_{\nu_{min}}^{\nu} j_\nu \, d\nu \Big/ \int_{\nu_{min}}^{\nu_{max}} j_\nu \, d\nu$$

THE ENERGY PACKETS' TRAJECTORIES

L_ν

Must iterate:
trajectories depend on temperature–dependent opacities and emissivities!!!

SED

ENERGY PACKETS

- The radiation field is expressed in terms of monochromatic packets of constant energy (Abbot & Lucy, 1985)

$$E(\nu) = n \bullet h\nu = E_0$$

- Every absorption is immediately followed by a re-emission of a packet with frequency given by the local dust or gas emissivity

  →**strict energy conservation imposed at each point in the region**

THE RADIATION FIELD

- In each grid cell the mean intensity of the radiation field can be expressed as (Lucy, 1999)

$$J_\nu = \frac{1}{4\pi}\frac{E_0}{\Delta t}\frac{1}{V}\sum_{d\nu} l$$

where $$\frac{E_0}{\Delta t} = \frac{L_*}{N}$$

V is the volume of the grid cell

l is the segment of trajectory within the grid cell

So if we can calculate the packets' trajectories (i.e. random walk), then we can automatically derive the mean intensity of the radiation field !!

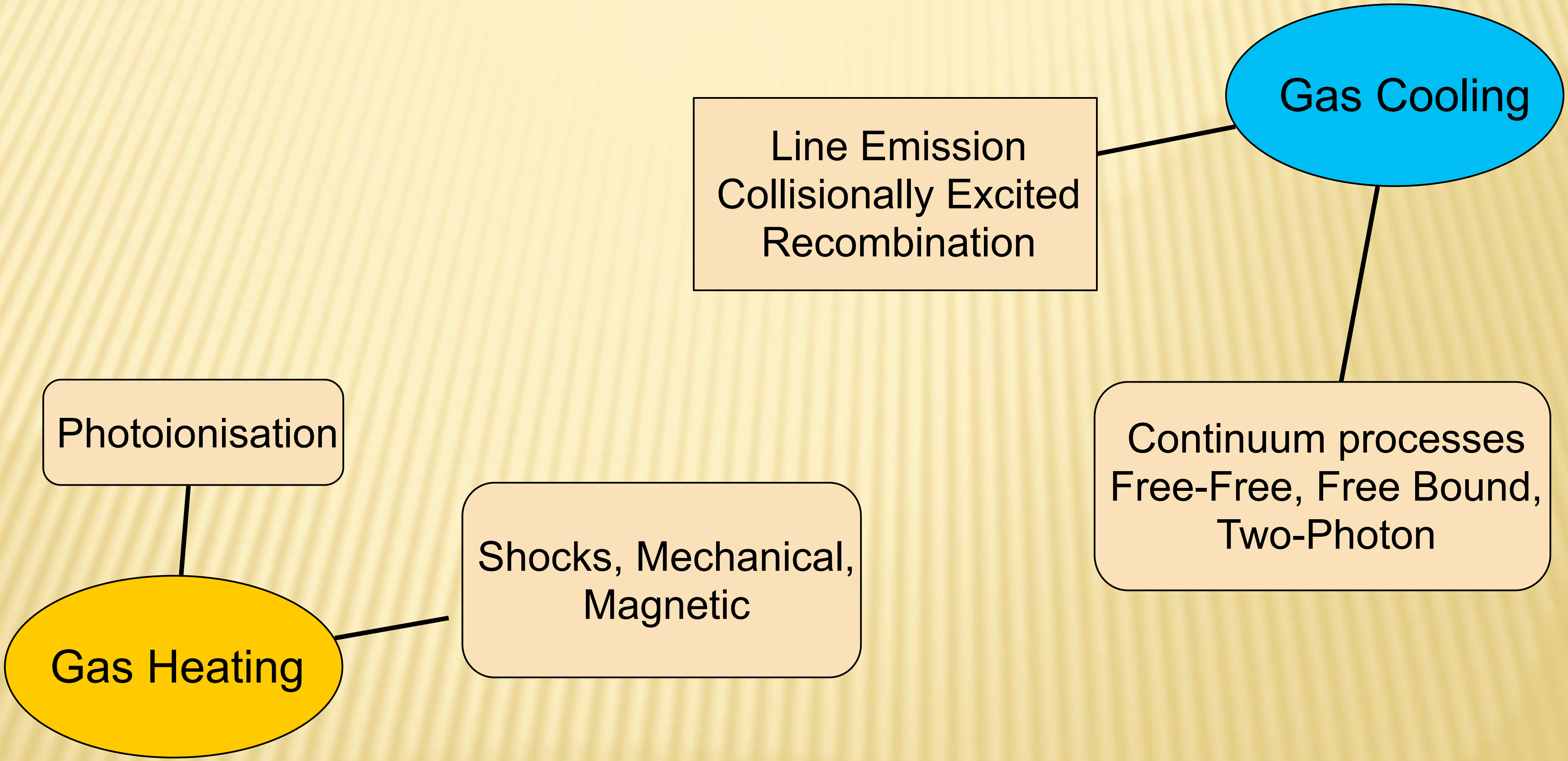
SUMMARY OF BASIC MONTE CARLO RT GAS & DUST

- Guess gas & dust temperatures and gas abundances

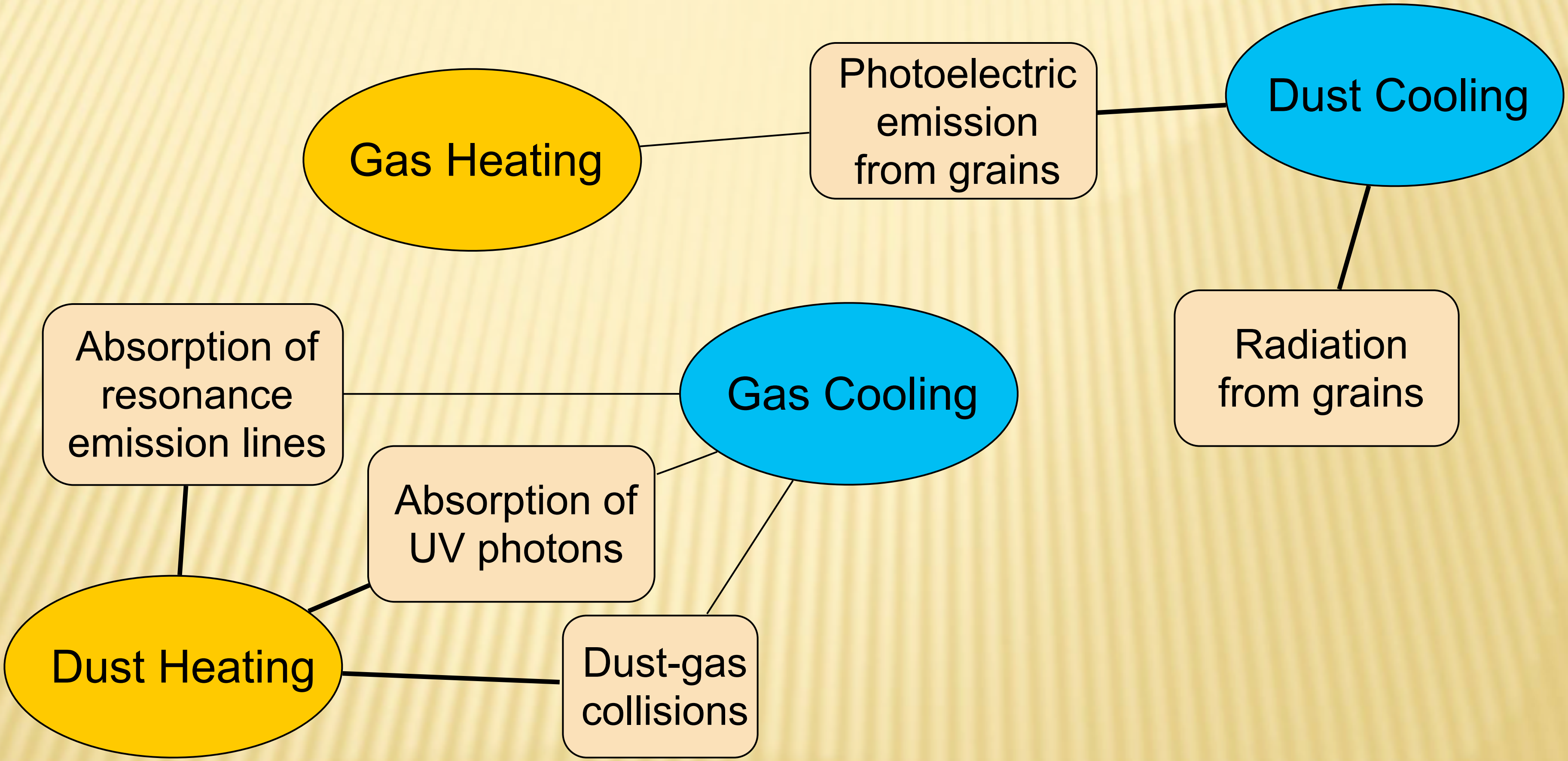
  ⟹ opacities and emissivities

- Packets trajectories ⟹ radiation field
- Ionization Balance/Chemistry ⟹ ion abundances, X
- Thermal Balance ⟹ gas & dust temperatures, Tg, Td
- Td+Tg+ X ⟹ opacities and emissivities

The (atomic/ionic) gas thermal balance (no dust)



Gas and Dust Interactions:
The dust thermal balance



Cloudy (Van Hoof et al., 2004, MNRAS 350, 1330)
Mocassin (Ercolano et al., 2005, MNRAS, 362, 1038)

MOnte CArlo SimulationS of Ionised Nebulae

Ercolano et al., 2003, 2005,2008 (www.3d-mocassin.net)

Version 2.02.70 of the code is public and parallelised (MPI)

…can treat…

- ✓Arbitrary geometries
- ✓Multiple grids of arbitrary resolution
- ✓Density &/or chemical inhomogeneities
- ✓Multiple/diffuse/non central ionising sources
- ✓3D photoionisation including X-ray &/or dust RT

…can provide…

- ✓Emission line intensity tables
- ✓Spectral energy distributions
- ✓3D (gas &/or dust) temperature distributions
- ✓3D ionisation structures
- ✓Emission line(s), continuum images

Voronoi–MOCASSIN

Hubber, Ercolano & Dales (2015, submitted)

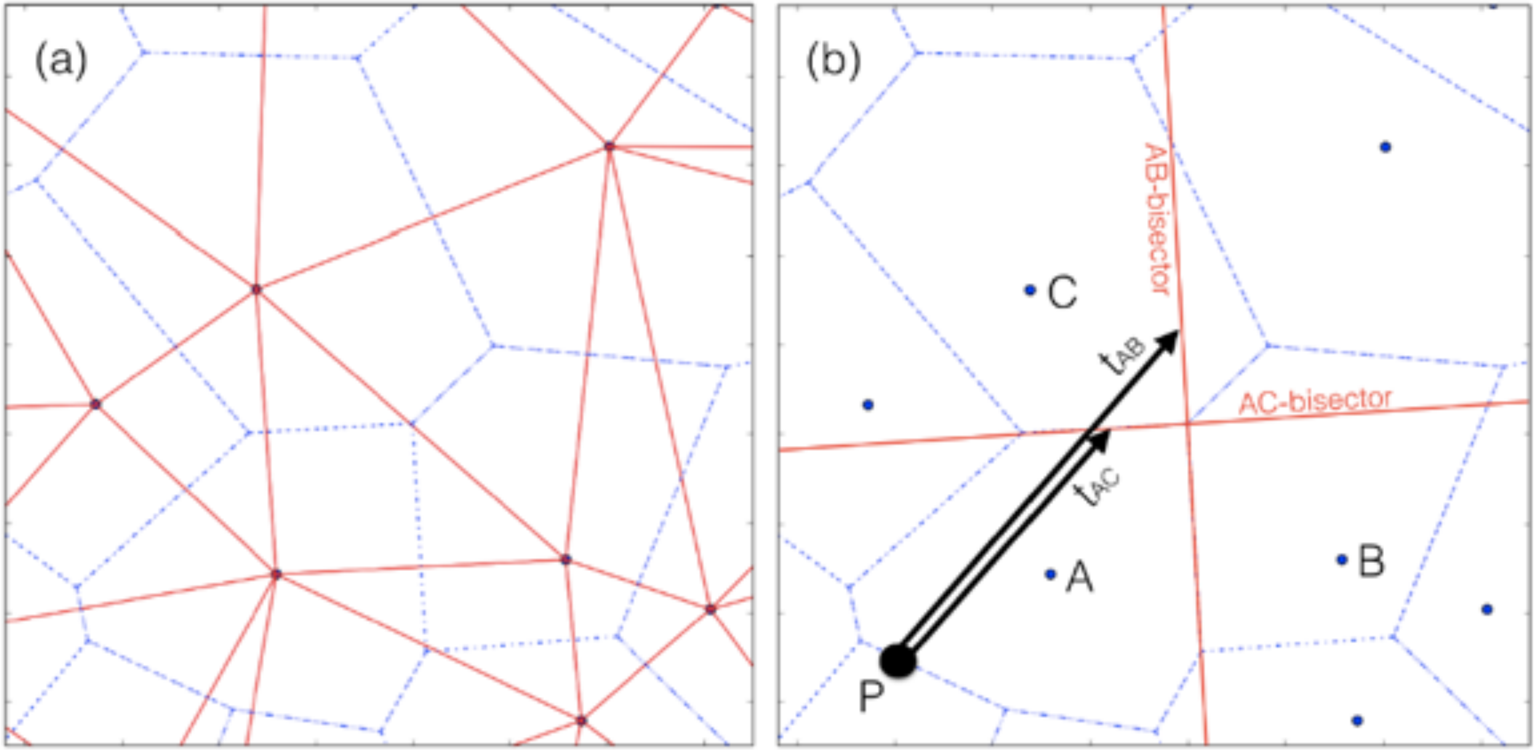


Figure 1. (a) Delaunay triangulation (red lines) and Voronoi tessellation (blue dot-dashed lines) for a selection of random points in 2D. (b) For a packet propagating through cell A originating at point P, we compute the distance the packet must propagate in order to intersect the point-point bisectors (which lie over the cell faces) of all neighbouring cells. For example, if we consider just cells B and C, we compute that the energy packet intersects the AC-bisector before the AB-bisector (i.e. $t_{AC} < t_{AB}$); therefore the energy packet next enters cell C at the intersection point.

Voronoi–MOCASSIN

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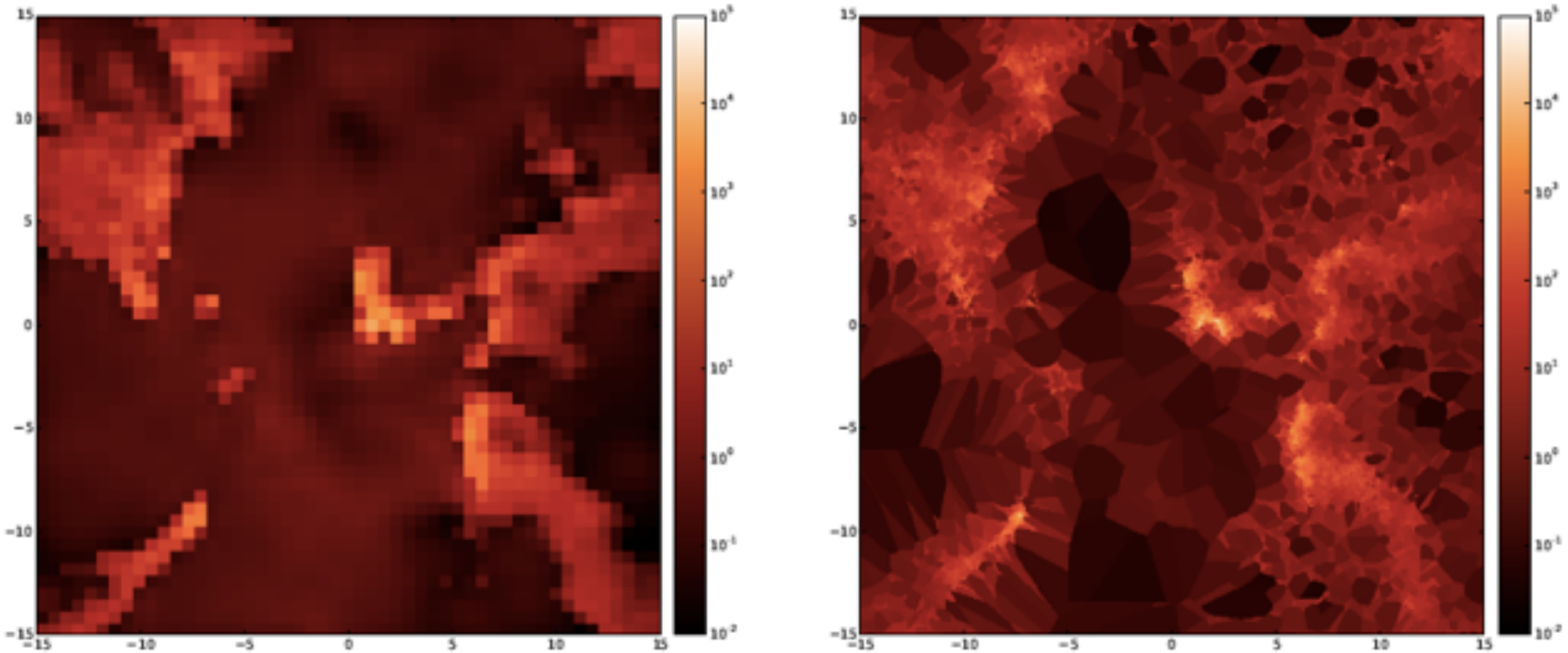


Figure 2. Number density slice (at $z = 0.0$) of atomic hydrogen (in cm^{-3}) from the ? simulation described in Section 4 for the Cartesian (left-hand panel) and the Voronoi (right-hand panel) versions of MOCASSIN. We note the far higher resolution in the dense filamentary structures for the Voronoi rendition for exactly the same number of cells. In contrast, the Cartesian version has unnecessary more resolution in the low density expanses in between the dense structures. Positions are measured in pc.

Voronoi–MOCASSIN

Hubber, Ercolano & Dales (2015, submitted)

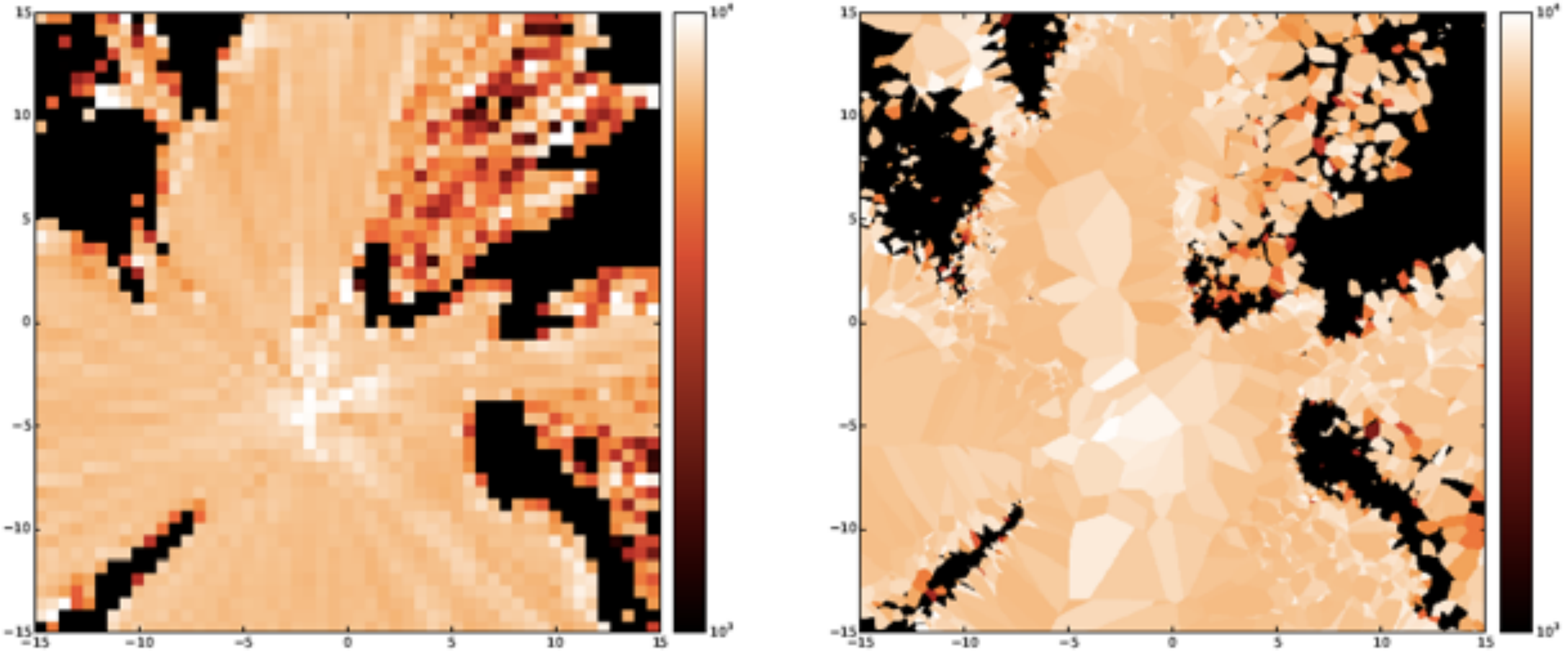


Figure 3. Gas temperature (in K) slice (at $z = 0.0$) of the ? simulation described in Section 4 for the Cartesian (left-hand panel) and the Voronoi (right-hand panel) versions of MOCASSIN. Both version produce the same large-scale features, particularly in the high-density/low-temperature filamentary structures which shield radiation from the stars. Positions are measured in pc.

Voronoi–MOCASSIN

Hubber, Ercolano & Dales (2015, submitted)

Line	Cartesian	Voronoi
Hβ / 10^{36} erg s^{-1}	3.74	3.77
Hβ 4861	1.0	1.0
He I 5876	0.0764	0.00939
N II 5755	0.0100	0.0127
N II 6548	0.419	0.446
N II 6584	1.28	1.36
O II 3726	1.20	1.62
O II 3729	1.57	2.09
O III 4363	0.00101	0.00201
O III 4932	0.0000309	0.0000671
O III 4959	0.0898	0.195
O III 5008	0.268	0.583
Ne III 3869	0.0106	0.0216
Ne III 3968	0.00320	0.00652
S II 4069	0.143	0.106
S II 4076	0.0497	0.0367
S II 6717	2.48	1.48
S II 6731	1.85	1.14
S III 6312	0.00575	0.00973
$\langle T[N_p N_e]\rangle$/K	7783	8330
$\langle He^+\rangle / \langle H^+\rangle$	0.15	0.32

Introduction to MOCASSIN

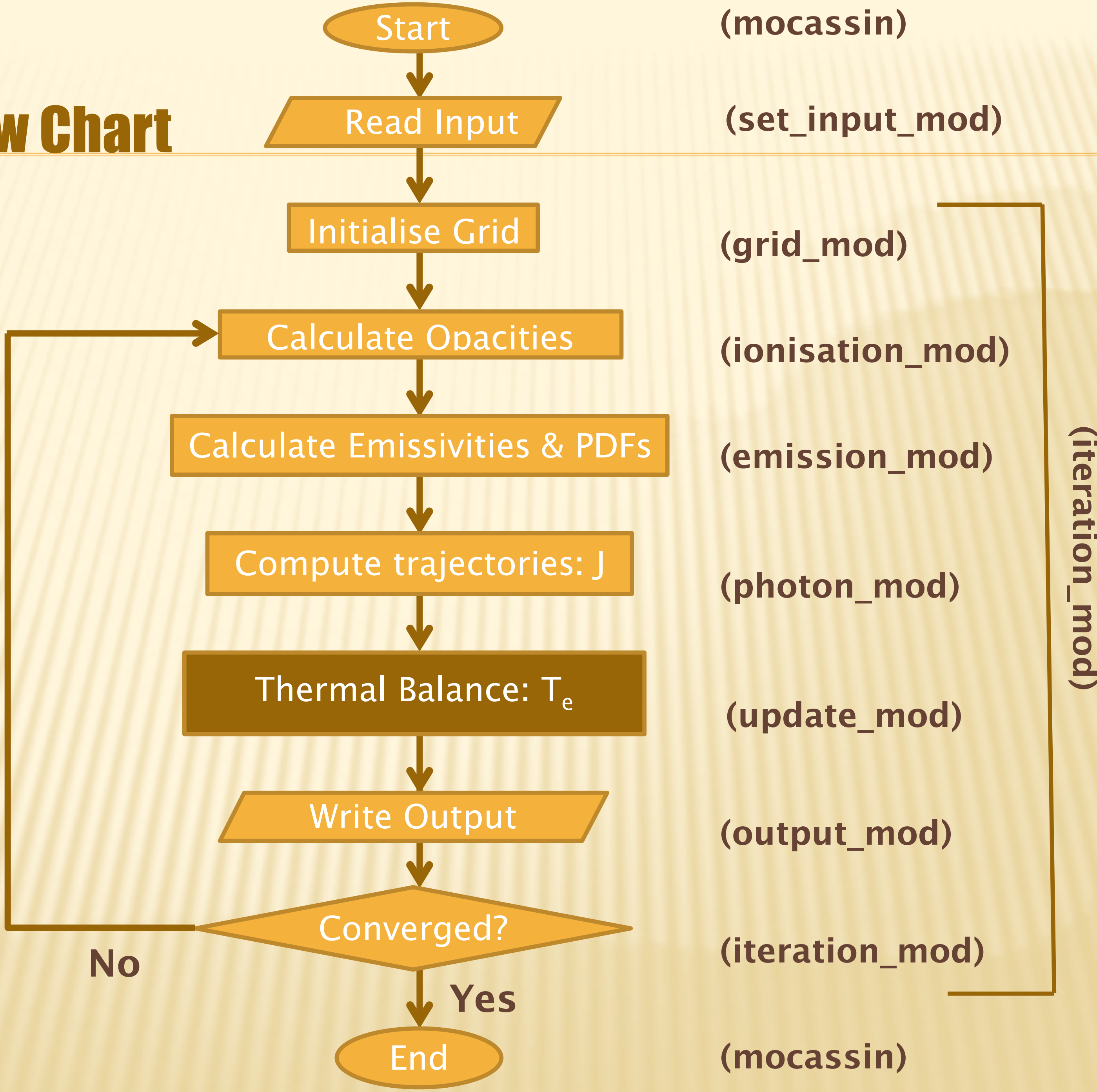
MOnte CArlo SimulationS of Ionised Nebulae

General Architecture

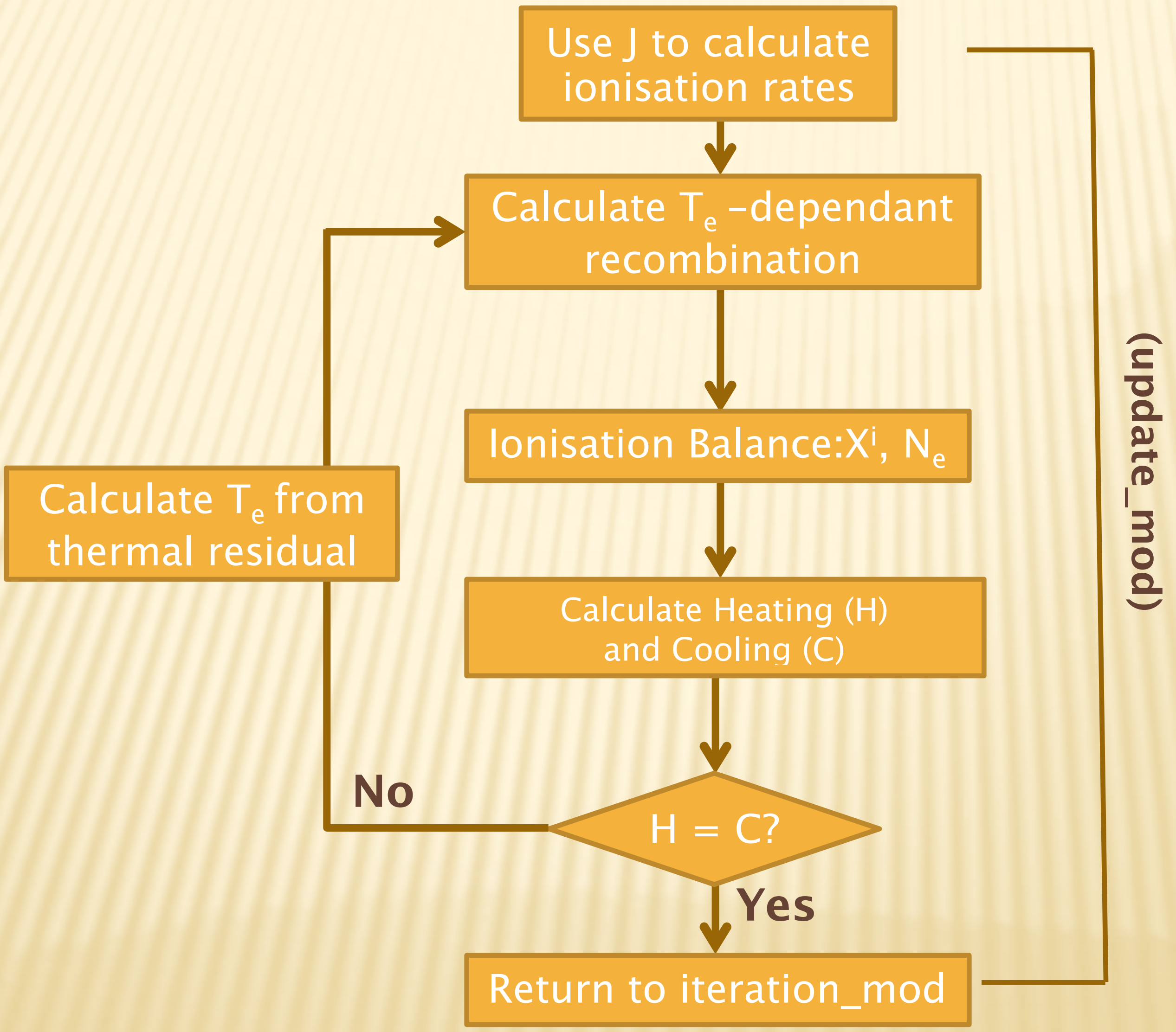
Inputs and Outputs

Benchmarks & Examples

MOCASSIN
Overall Flow Chart



Thermal & Ionisation Balance - Simple Flow Chart



MOCASSIN INSTALLATION

- Fortran 90 compiler (gfortran, free intel compiler -ifort)
- Message Passing Interface (MPI)
- Compile using makefile but…
  …<u>**DO NOT USE AGGRESSIVE OPTIMISATION (-O2,-O3)**</u>
- Directory Structure:
  - source/ the source modules
  - data/ the gas atomic data (mainly)
  - dustData/ the dust atomic data
  - input/ user's input files
  - output/ mocassin's output
  - benchmarks/ benchmarks' input/ and output/
  - examples/ special features example cases

MOCASSIN INPUTS – THE BASICS

- Talk to MOCASSIN through input/input.in
- Use the keywords listed in the manual

INPUT	PHYSICAL QUANTITIES	MOCASSIN KEYWORDS
Gas and/or dust density distribution	nH [cm−3], Md/Mg or Nd [cm−3]	densityFile, Hdensity, MdMg, MdMh, Ndust
Gas and/or dust chemical composition	A/H (by number) Grain Chemistry & Size	nebComposition, dustFile
Irradiating Sources	F_{λ} (location)	contShape, LStar, Lphot
Atomic, Ionic and dust data	Too many!!!!	data/ dustData/

MOCASSIN OUTPUTS– THE BASICS

- All output files are in the output/ directory
- Run-time messages sent to screen (pipe to log)

OUTPUT	PHYSICAL QUANTITIES	OUTPUT FILE
Gas and/or dust temperature	T_e	grid1.out, temperature.out, dustGrid.out
Gas ionisation structure	$X^i/X, <X$	grid2.out, ionratio.out
Continuum Emission	λF_λ	SED.out
Emission Line Spectrum	L_λ	lineFlux.out

THE GAS BENCHMARKS

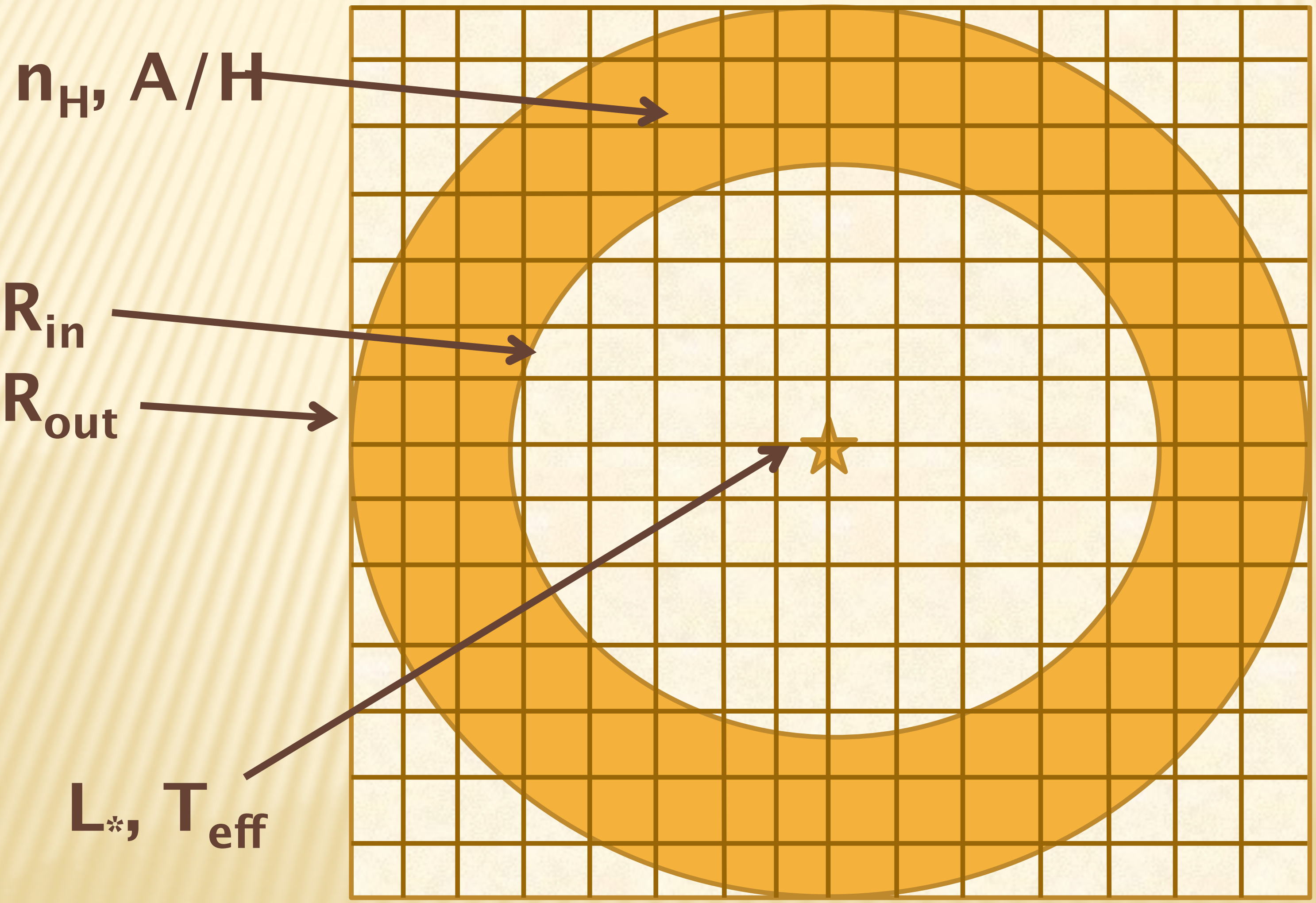
- Based on the benchmarks deviced in the Meudon/Lexington workshops (e.g. Pequignot et al 2001, Ercolano et al. 2003)
- Typical planetary nebulae and HII region conditions

Table 1. Lexington 2000 benchmark model input parameters.[a]

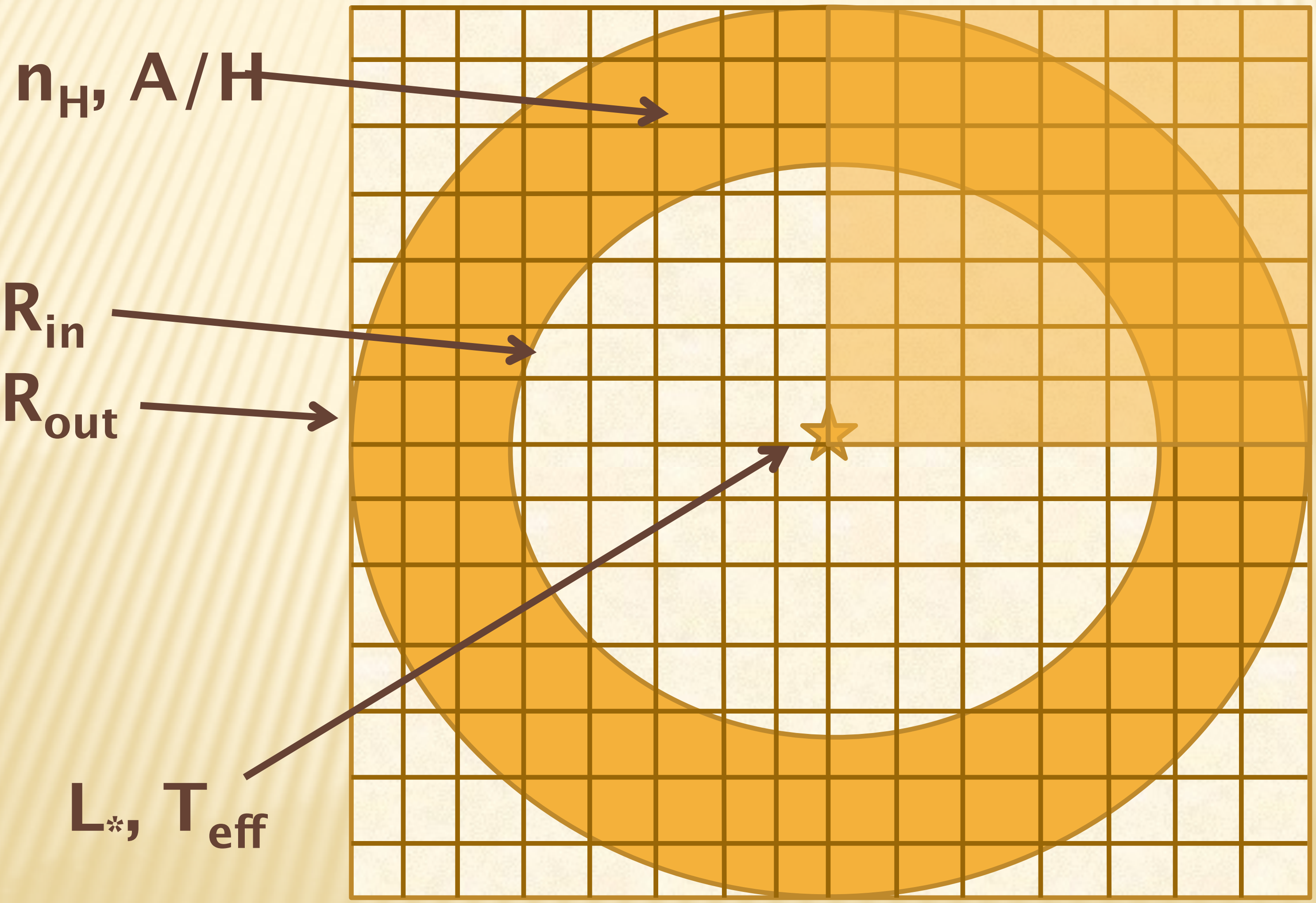
Parameter	HII40	HII20	PN150	PN75
$L(\mathrm{BB})/10^{37}$ erg s^{-1}	308.2	600.5	3.607	1.913
$T(\mathrm{BB})/10^{3}$ K	40	20	150	75
$R_{\mathrm{in}}/10^{17}$ cm	30	30	1	1.5
$n_{\mathrm{H}}/\mathrm{cm}^{-3}$	100	100	3000	500
He/H	0.10	0.10	0.10	0.10
C/H $\times 10^5$	22	22	30	20
N/H $\times 10^5$	4	4	10	6
O/H $\times 10^5$	33	33	60	30
Ne/H $\times 10^5$	5	5	15	6
Mg/H $\times 10^5$	–	–	3	1
Si/H $\times 10^5$	–	–	3	1
S/H $\times 10^5$	0.9	0.9	1.5	1

[a] Elemental abundances are by number with respect to H.

THE GAS BENCHMARKS *(CONTINUED)*



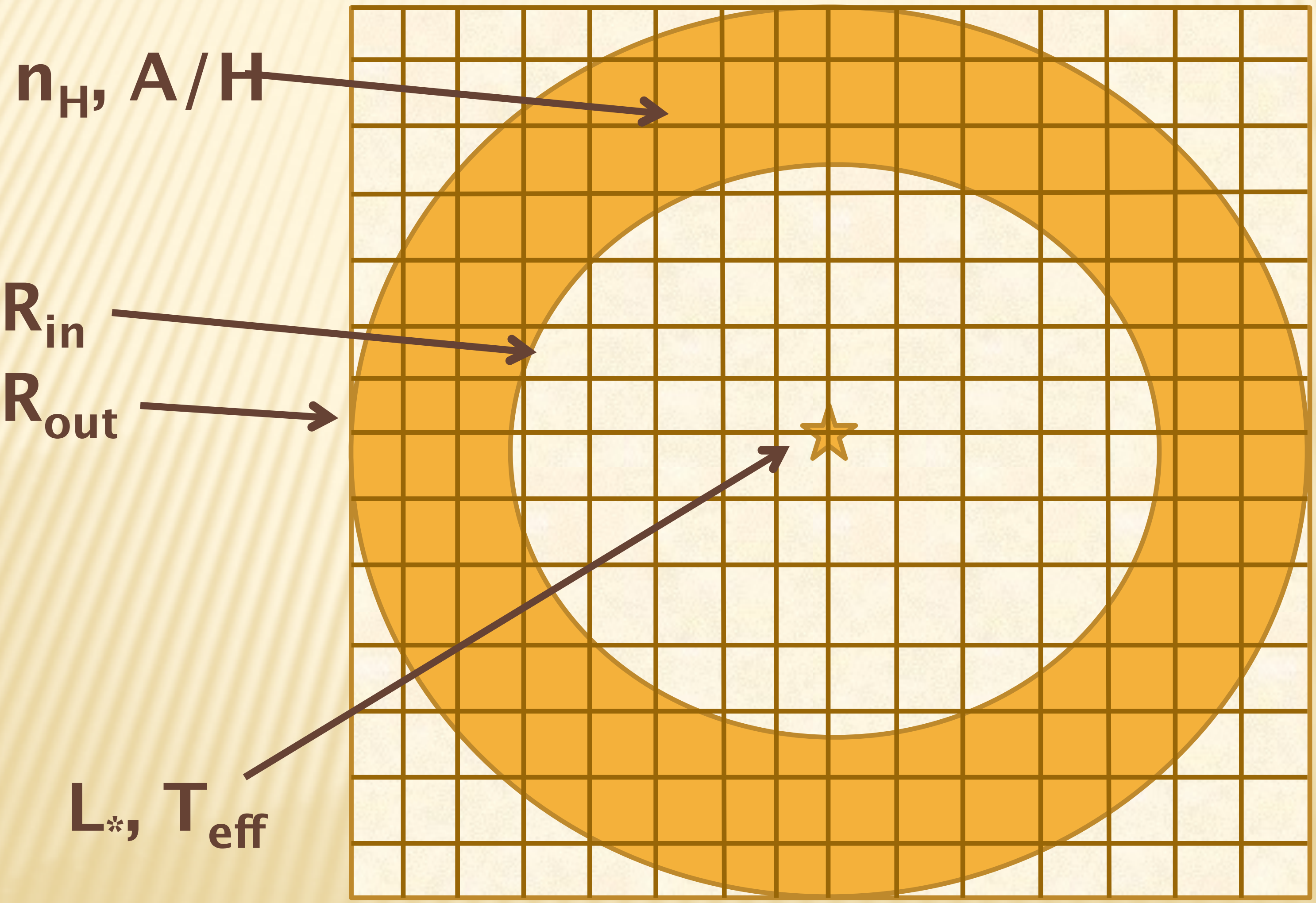
THE GAS BENCHMARKS *(CONTINUED)*

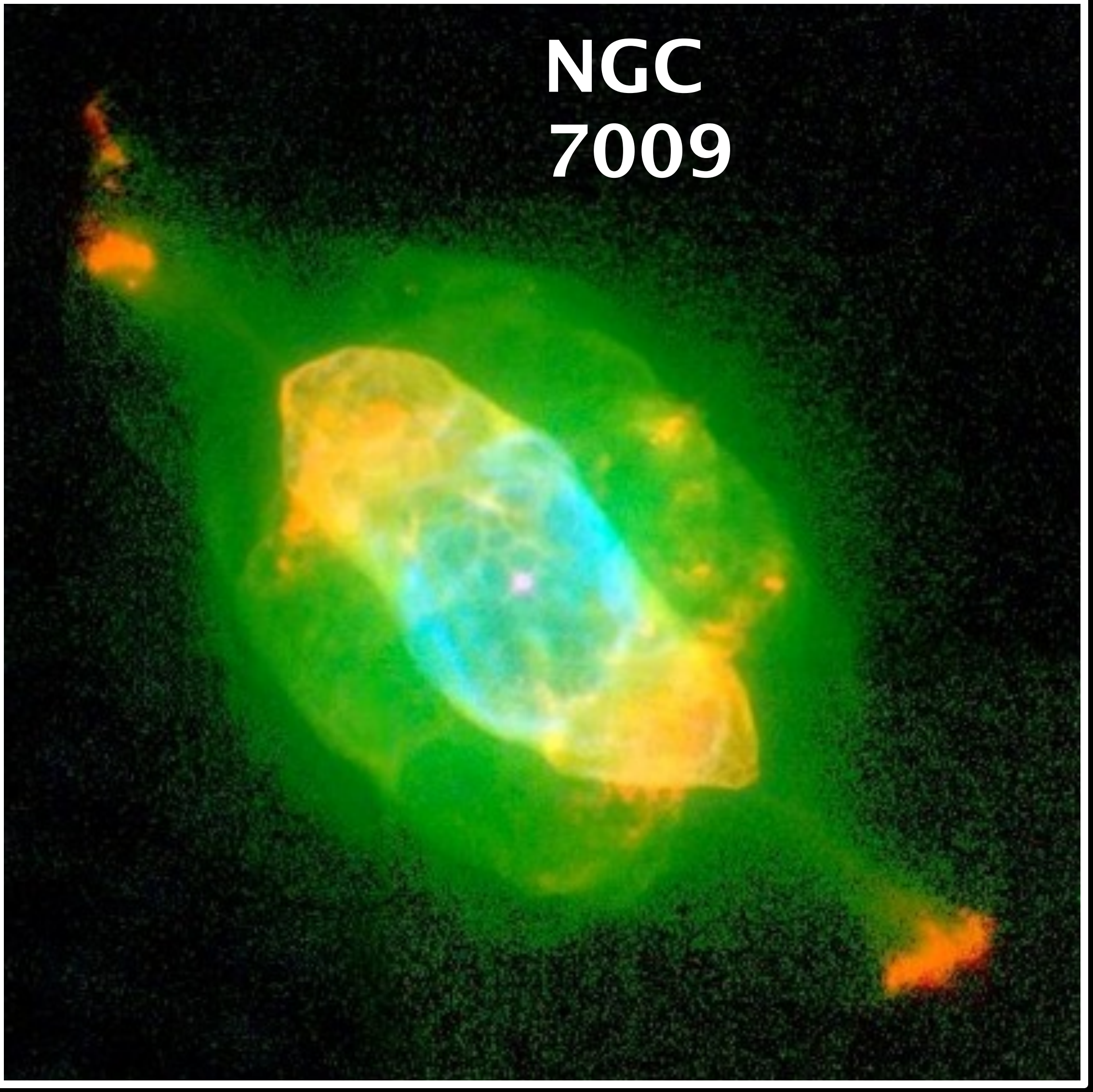


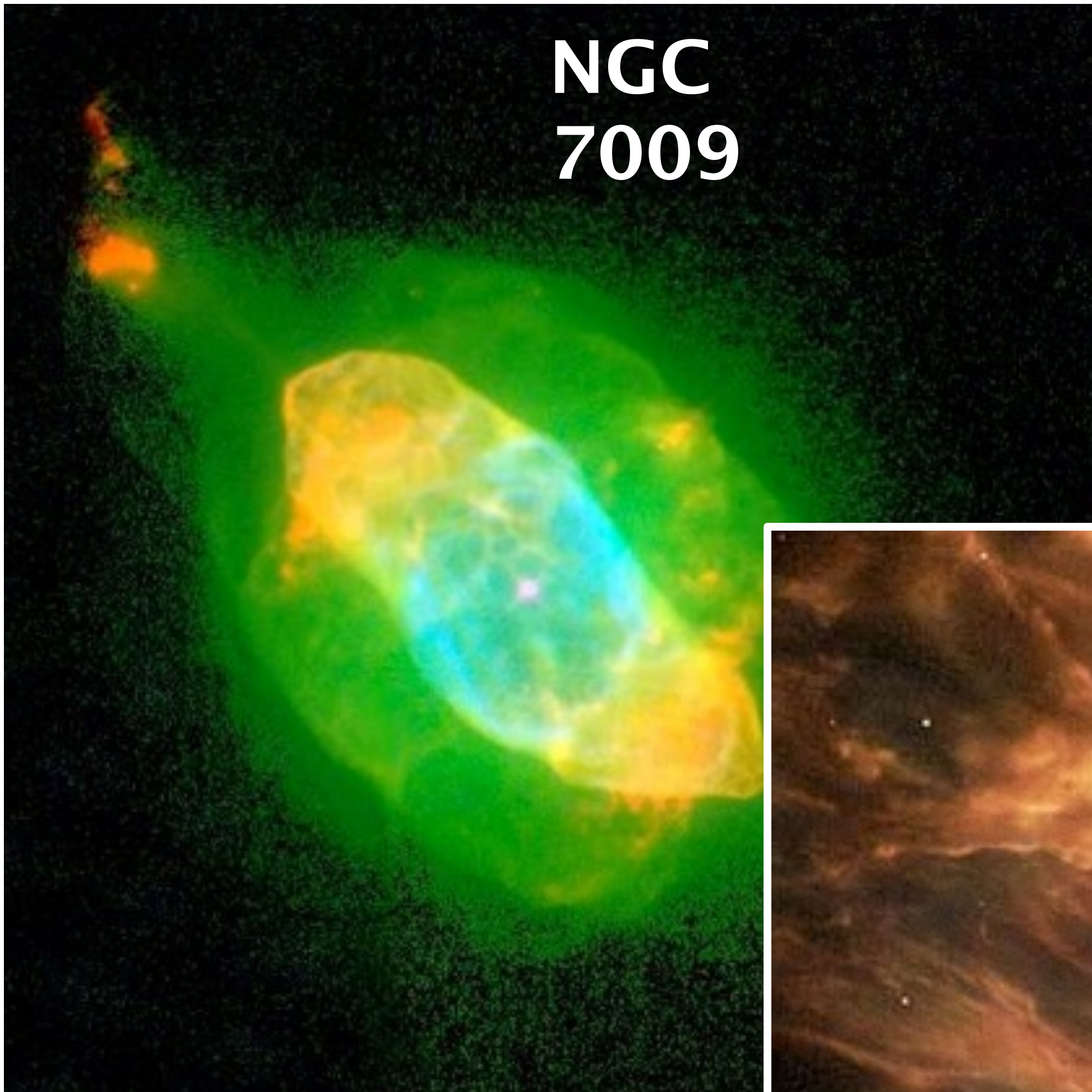
Modelling an ionised region
-basic steps-

1. **The density distribution** (setting up a grid)
2. **The elemental abundances** (inhomogeneities?)
3. **The ionising spectrum** (single or multisources)
4. **Comparing with the observations**

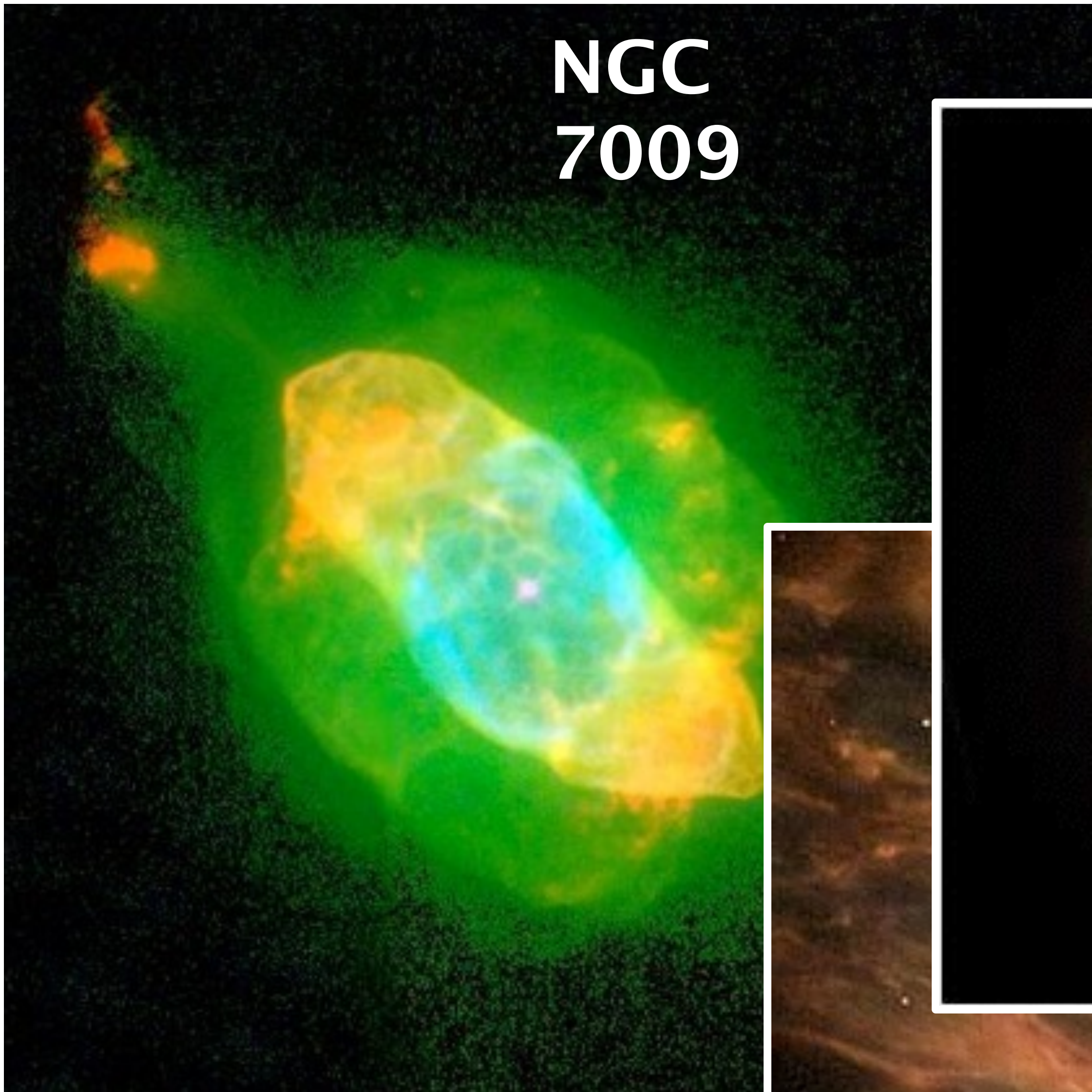
THE GAS BENCHMARKS




NGC
7009

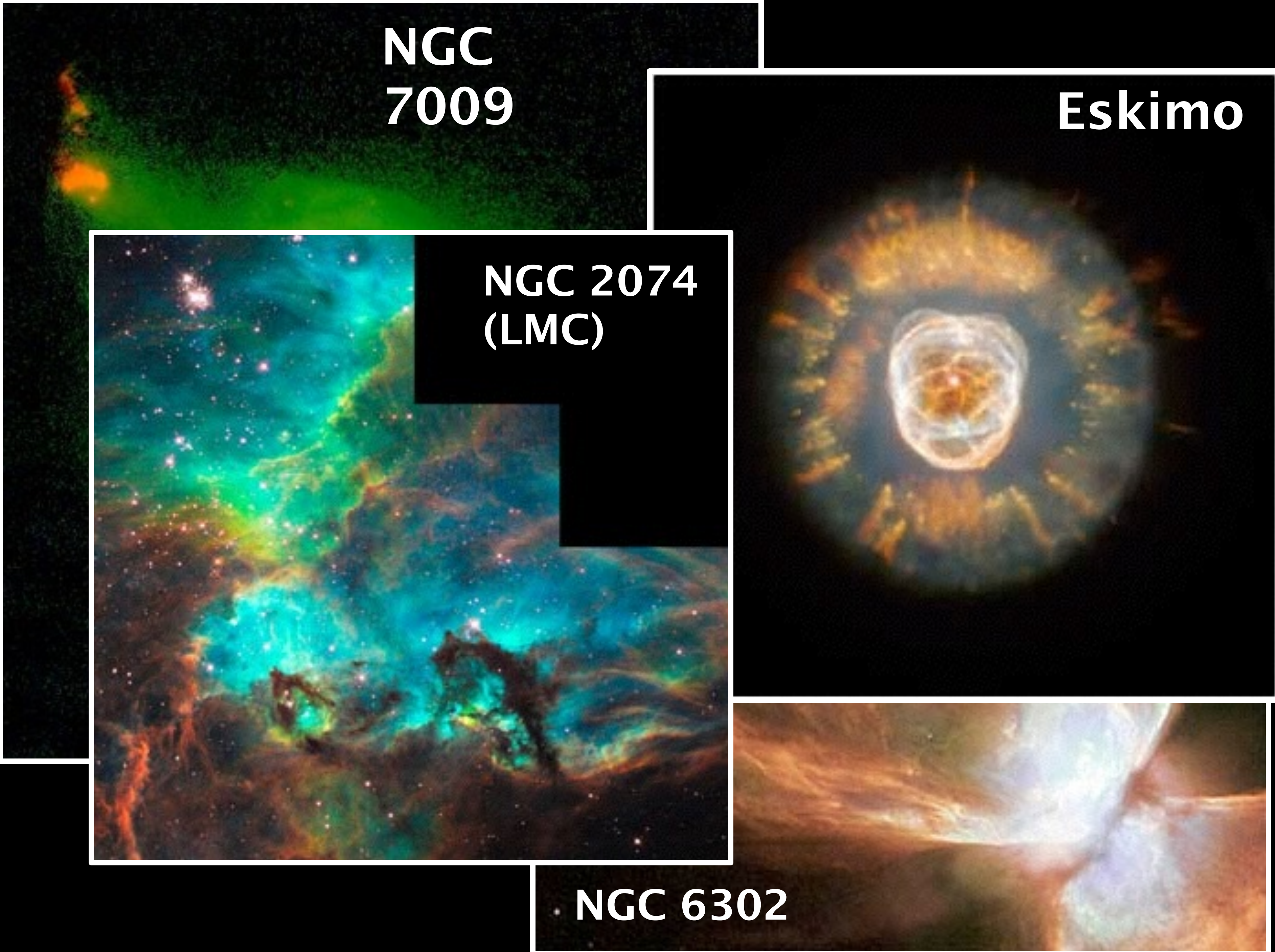

NGC
7009

NGC 6302


NGC
7009


Eskimo


NGC 6302


NGC 7009
Eskimo
NGC 2074 (LMC)
NGC 6302

Modelling an ionised region
-basic steps-

1. The density distribution (setting up a grid)

2. The elemental abundances (inhomogeneities?)

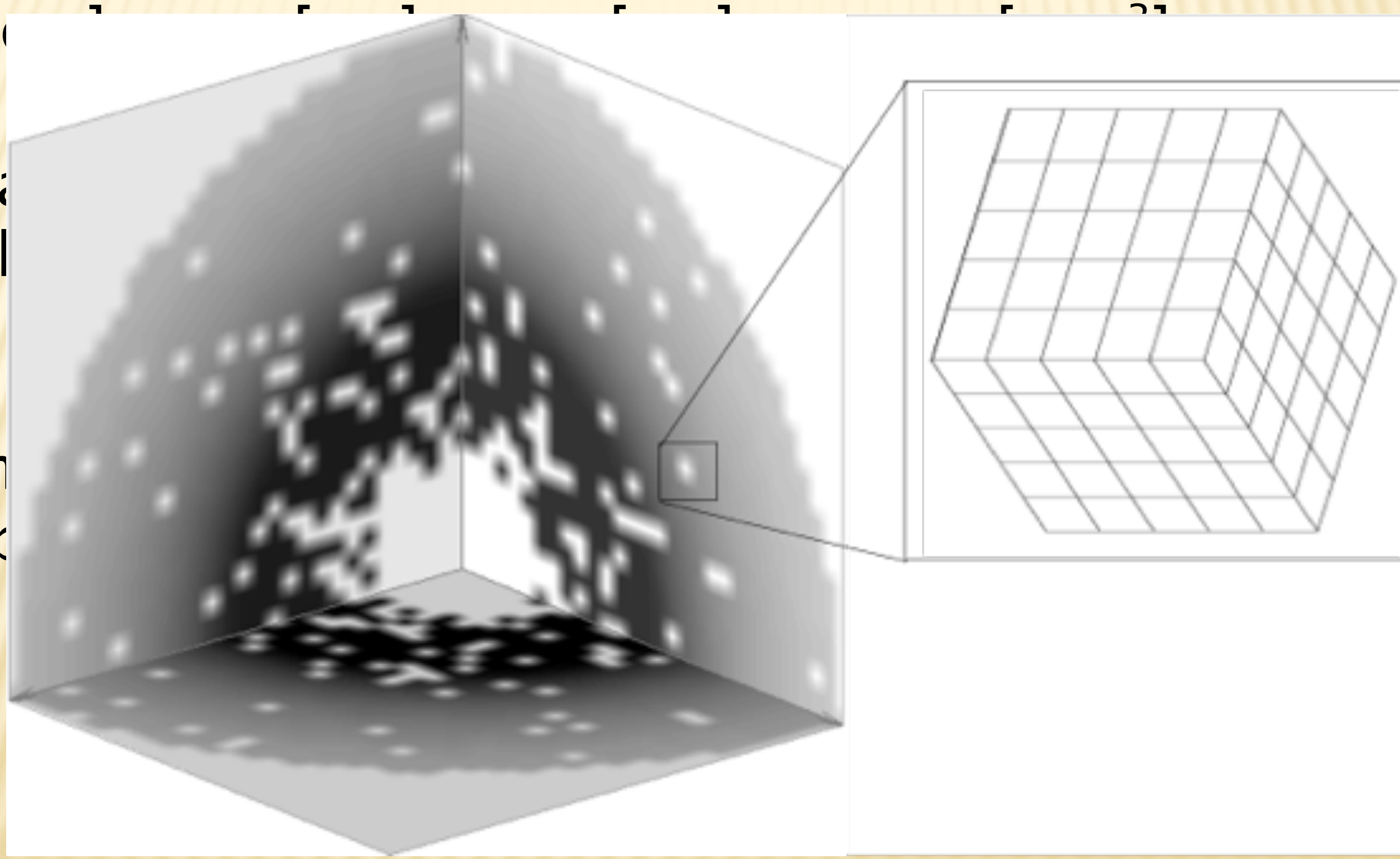
3. The ionising spectrum (single or multisources)

4. Comparing with the observations

1. THE DENSITY DISTRIBUTION

•Make the Cartesian grid as an ascii table of form

x [



•If axi ... be

model

•Axes ... be

obtain ... gas &

examp

1. THE DENSITY DISTRIBUTION

•Make the Cartesian grid as an ascii table of form
x [cm] y [cm] z [cm] n_H [cm^{-3}]

•If axial symmetry only 1/8th of the nebulae needs to be modeled (symmetricXYZ)

•Axes spacing are arbitrary – multiple resolutions can be obtained with multiple grids (see examples/multigridgas & examples/multigridgasdust)

•2D grids are also allowed in this case the y column should be included with all zero's

•Gas and dust can be defined independently or via a dust-to-gas ratio

Modelling a PN or HII region -basic steps-

1. The density distribution (setting up a grid)
2. The elemental abundances (inhomogeneities?)
3. The ionising spectrum (single or multisources)
4. Comparing with the observations

2. ELEMENTAL ABUNDANCES

- Always include all more abundant elements
  - important for the thermal balance (e.g. H, He, C, N, O, Ne, S)

- Chemical inhomogeneities included by defining multiple zones
  - see multiChemistry keyword.

Modelling a PN or HII region
-basic steps-

1. The density distribution (setting up a grid)

2. The elemental abundances (inhomogeneities?)

3. The ionising spectrum (single or multisources)

4. Comparing with the observations

3. THE IONISING

- Use stellar atmosphere models for central star PNe (e.g. Rauch models, http://astro.uni-tuebingen.de/~rauch/)

- Use cluster or single OB star models for HII regions (e.g. Starburst99, http://www.stsci.edu/science/starburst99/)

- Use any input spectrum as an ascii table of
  Wavelength [A]   Eddington fluxes [erg/cm^2/s/A/sr]

- Multiple ionisation sources and non-central locations available (multiPhotoSources see also examples/multistars)

Modelling a PN or HII region
-basic steps-

1. The density distribution (setting up a grid)

2. The elemental abundances (inhomogeneities?)

3. The ionising spectrum (single or multisources)

4. Comparing with the observations

4. COMPARING WITH THE OBSERVATIONS

- Emission line spectrum
  - Integrated over all volume (default; lineFlux.out)
  - Integrated through a slit (slit)
  - Integrated through an arbitrary aperture (mocassinPlot)

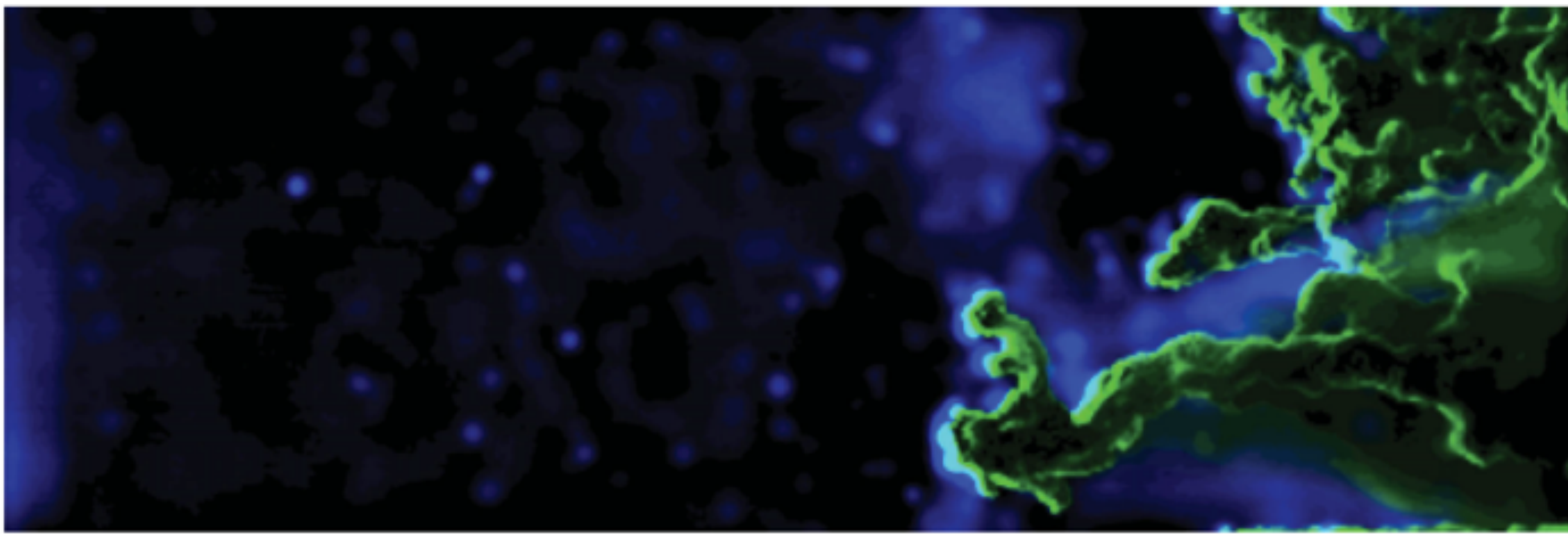
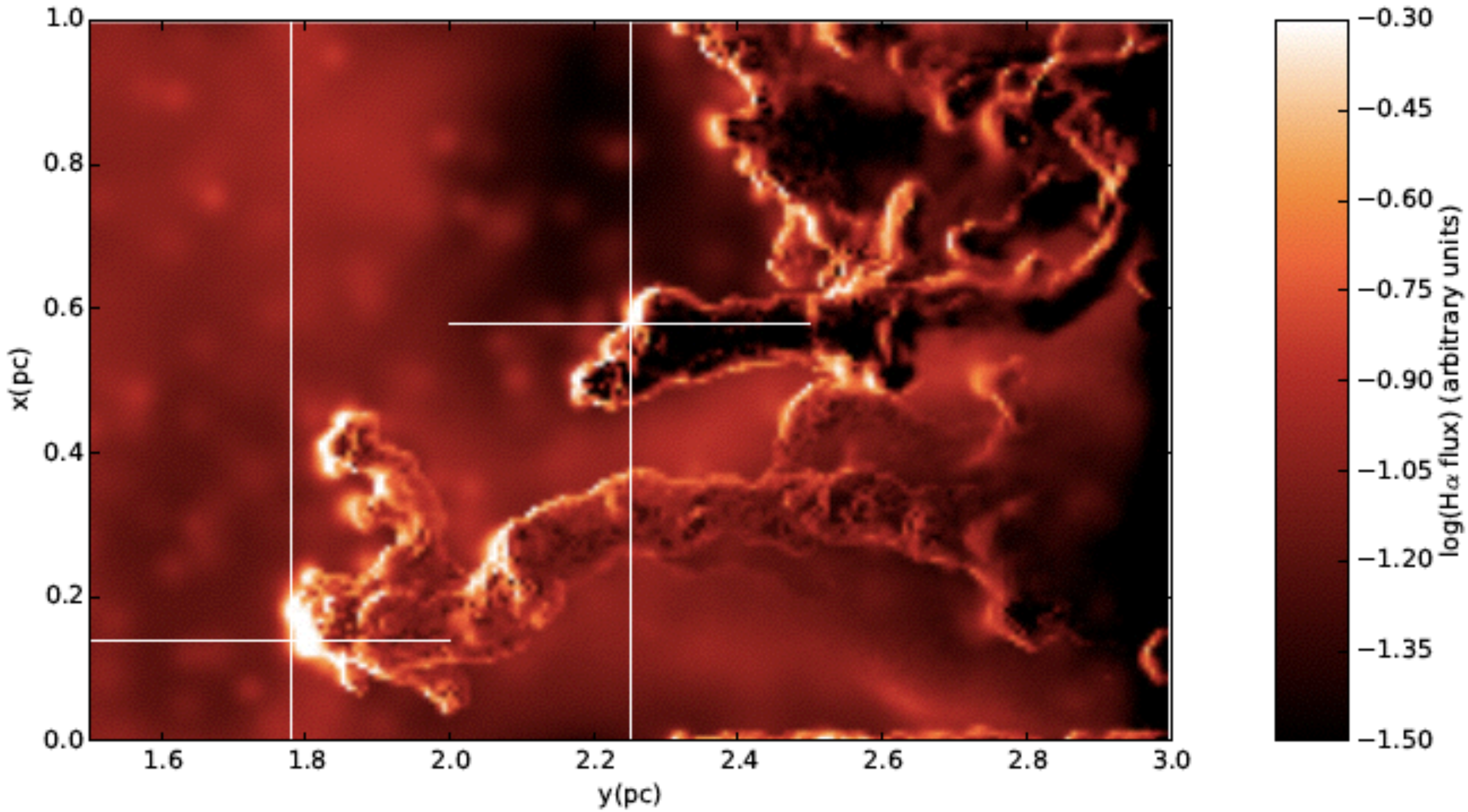


Figure 1. False colour composite image of the EG11 pillar at $t = 500$ kyr, where red is Hα, blue is [O III] $\lambda\lambda$5007, 4959 and green is a combination of the two lines.

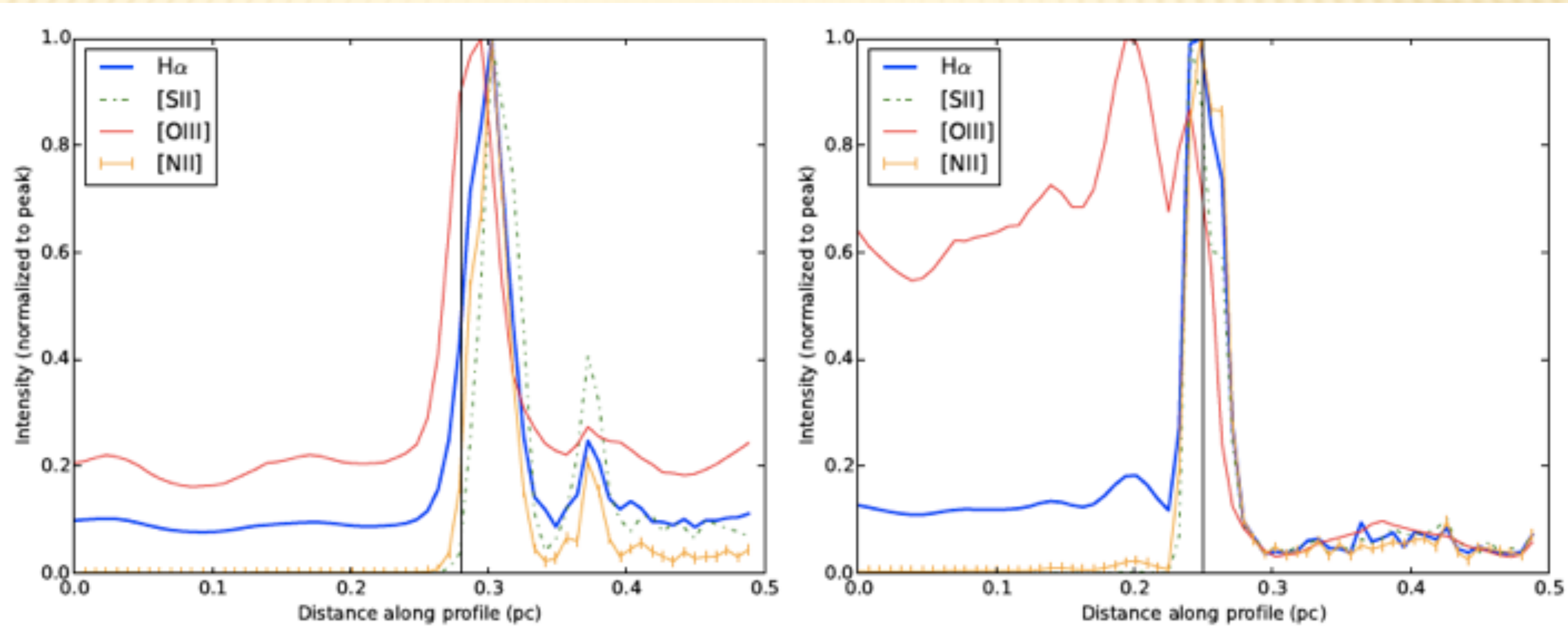
Pillars of Creation Ercolano et al. (2012)

4. COMPARING WITH THE OBSERVATIONS



Pillars of Creation McLeod et al. (2015)

4. COMPARING WITH THE OBSERVATIONS



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