Molecular line radiative transfer simulations of prestellar objects

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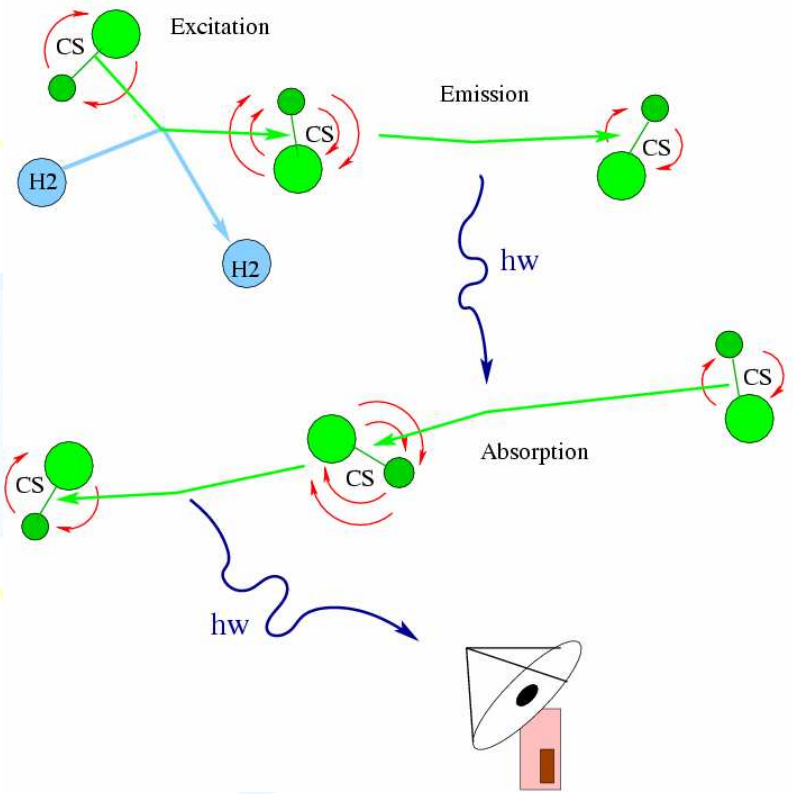
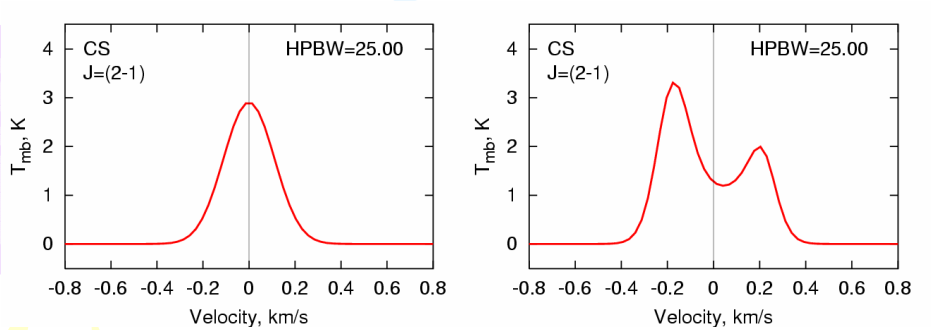
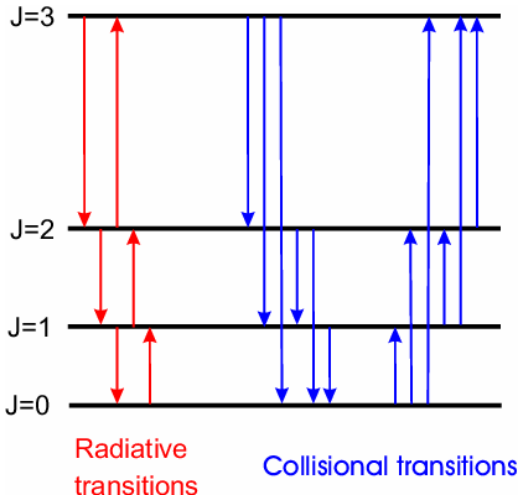
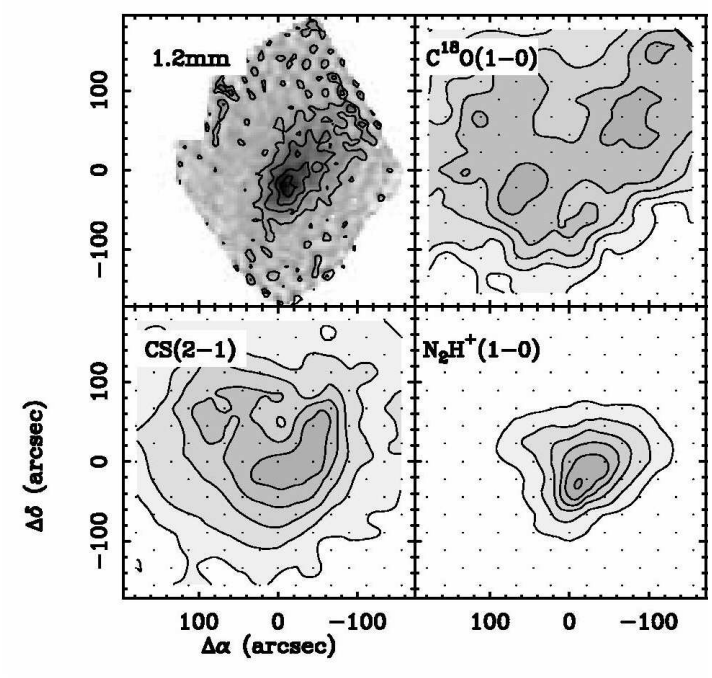
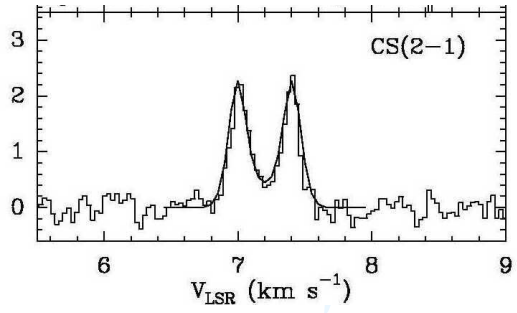


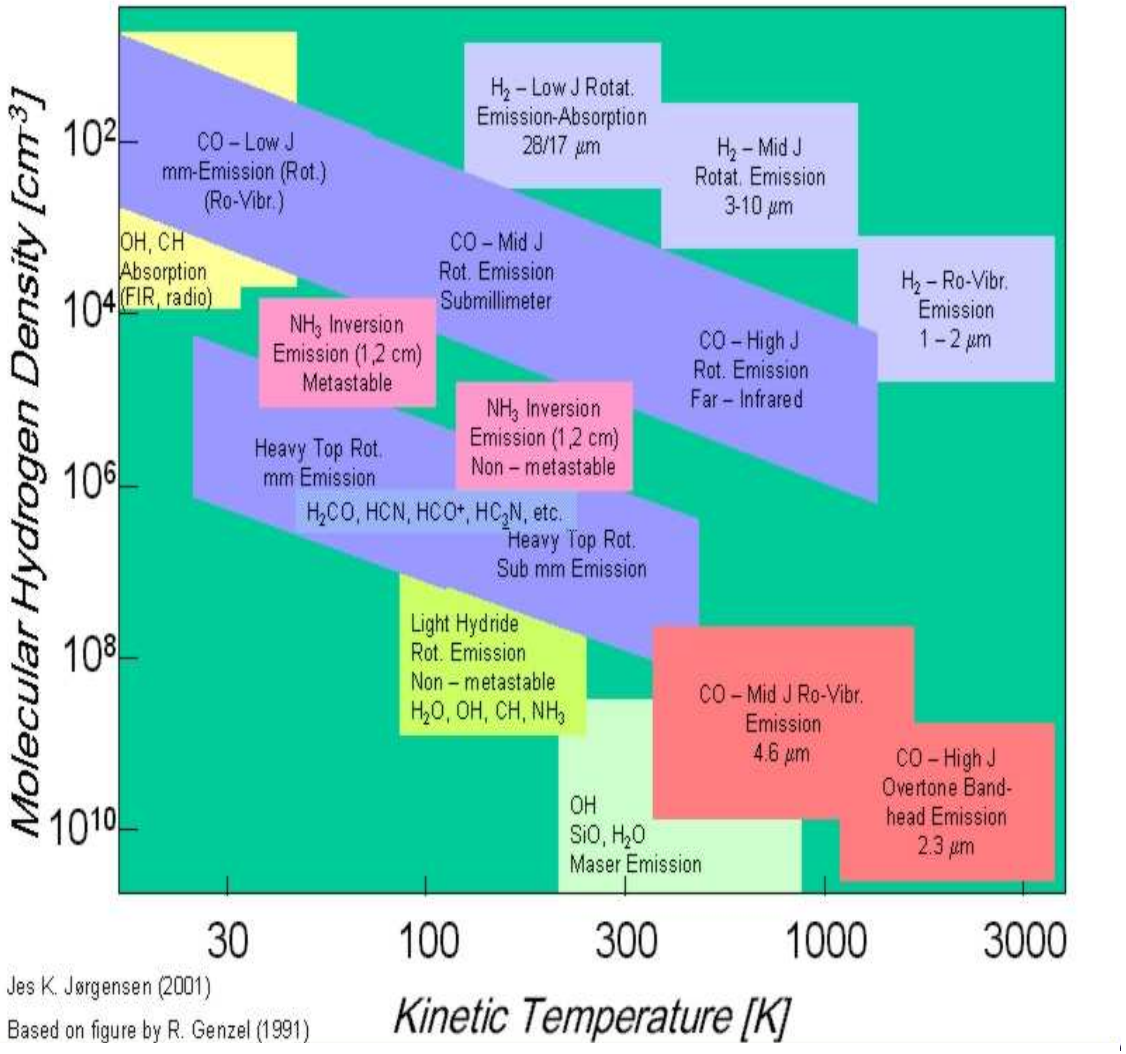




Why are the molecular lines so important?







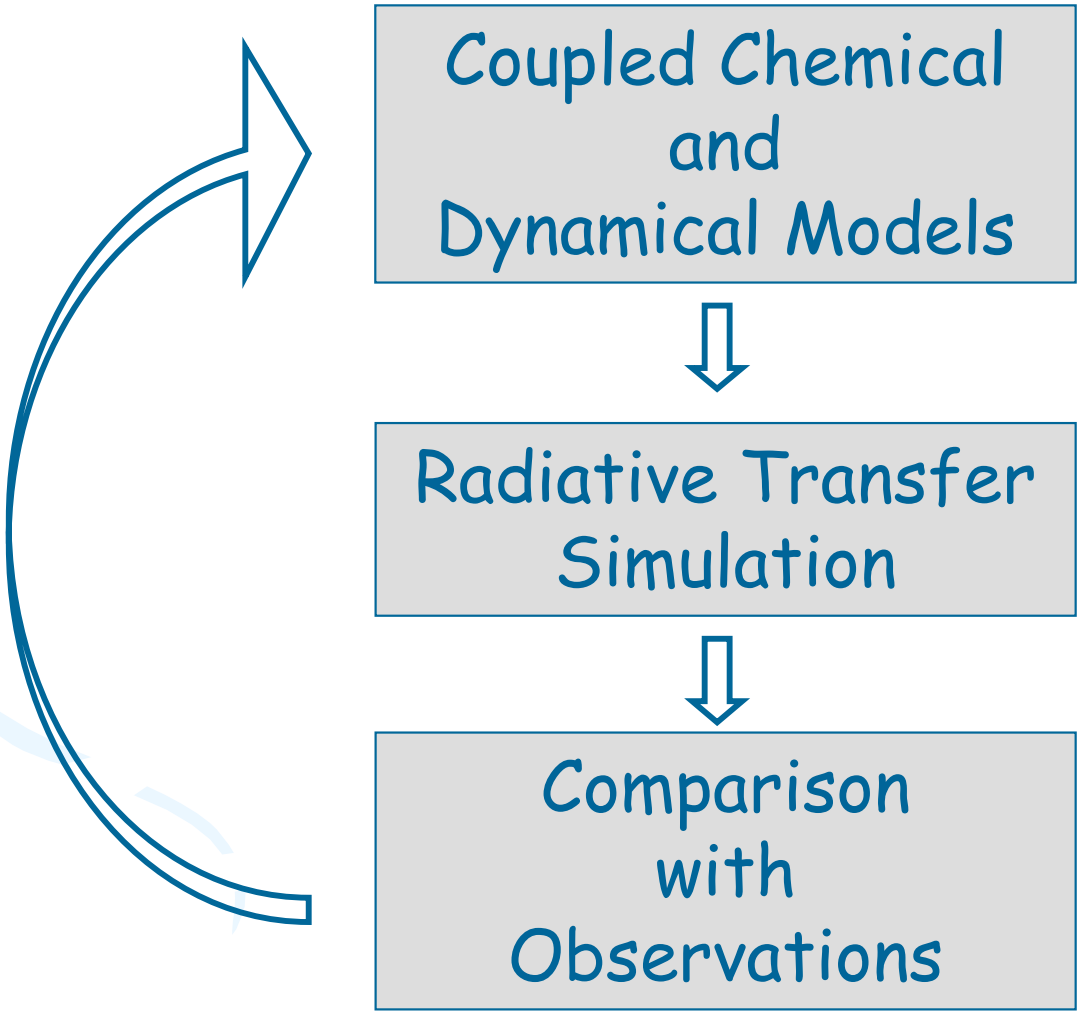
Molecular line observations allow to study physical conditions and kinematics of prestellar objects!

What are the problems with molecular lines ?

Chemical structure of the prestellar objects can be complex

Non-LTE conditions of the molecular line generation

How to extract information then from molecular lines?



1. Introduction to LRT numerical simulations

- Concept of the LRT simulations
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Equations of LRT

$$\frac{dI_\nu}{ds} - -\alpha_\nu I_\nu + j_\nu, \tag{1}$$

and a balance equation for the energy-level populations,

$$n_u \left[\sum_{l<u} A_{ul} + \sum_{l\neq u} (B_{ul}\overline{J}_{ul} + C_{ul}) \right] \tag{2}$$
$$= \sum_{l>u} n_l A_{lu} + \sum_{l\neq u} n_l (B_{lu}\overline{J}_{ul} + C_{lu}),$$

where I_ν is the spectral intensity of the radiation and n_k are the level populations. Equations (1) and (2) are related by the emission and absorption coefficients,

$$j_\nu^{ul} - \frac{h\nu_{ul}}{4\pi} n_u A_{ul} \phi_{ul}(\nu), \tag{3}$$

$$\alpha_\nu^{ul} = \frac{h\nu_{ul}}{4\pi} (n_l B_{lu} - n_u B_{ul}) \phi_{ul}(\nu), \tag{4}$$

and by the mean intensity of the radiation $\overline{J}_{ul}$, which is defined by the expression

$$\overline{J}_{ul} = \frac{1}{4\pi} \int_{4\pi} d\Omega \int_0^\infty I_\nu \phi_{ul}(\nu) d\nu. \tag{5}$$

In these formulas, A_{ik} and B_{ik} are the Einstein coefficients; C_{ik}, the coefficients for collisional excitation; ul, indices specifying the transition $u \rightarrow l$; and $\phi_{ul}(\nu)$, the line profile function, which is defined in the approximation of total redistribution over frequency and a Maxwellian turbulence spectrum as

$$\phi_{ul}(\nu) = \frac{c}{b\nu_{ul}\sqrt{\pi}} \tag{6}$$
$$\times \exp\left(-\frac{c^2(\nu - \nu_{ul} - (\mathbf{v}\cdot\mathbf{n})\nu_{ul}/c^2)}{\nu_{ul}^2 b^2} \right).$$

Here, ν_{ul} is the central frequency of the transition $u \rightarrow l$; $\mathbf{v}$, the regular velocity; $\mathbf{n}$, a unit vector in the direction of the photon's propagation; and b, a parameter that is related to the kinetic temperature T_k and the most probable value of the microturbulent velocity V_t by the expression

$$b^2 = \sqrt{\frac{2kT_k}{m_{mol}} + V_t^2}. \tag{7}$$

Basic assumptions:

- Stationary state
- Full frequency redistribution
- Micro-turbulence

Difficulties:

- Non-linear integro-differential system of equations
- Non-local problem, where the cells are globally coupled
- In general, 6D problem

2D NLTE code "URANIA"

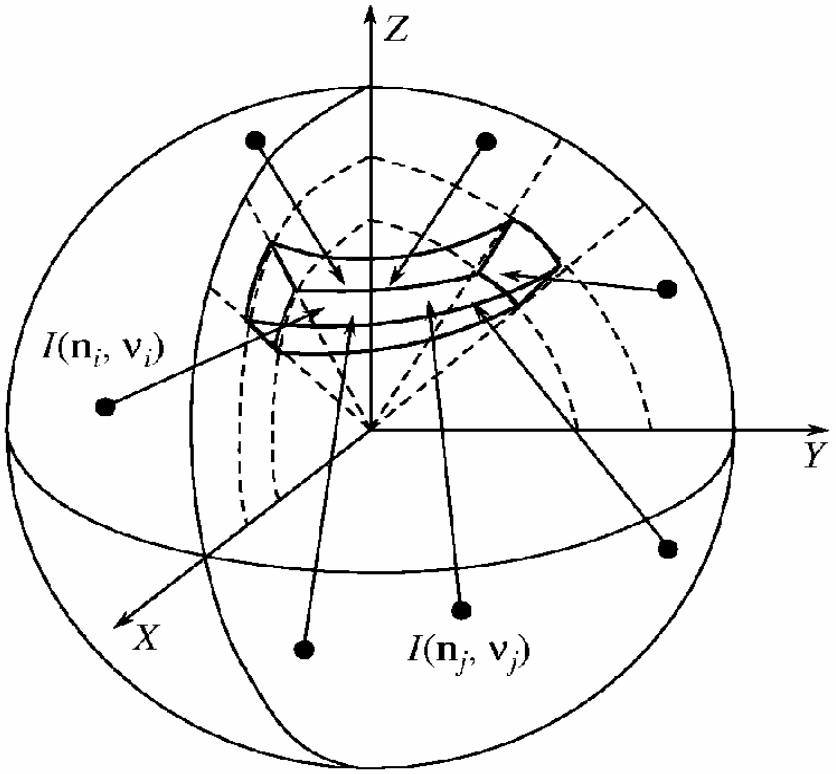


Fig. 1. Schematic of the computation of the mean radiation intensity (in a spherical coordinate system). The bold lines show the borders of an elementary cell. The rays show random directions for the integration of the transfer equation (1) for the given cell. The initial points for the integration (arrows) are randomly distributed inside the cell. The integration along each ray is continued to the boundary of the cloud. The mean radiation intensity is defined as the average of $\{I_i\}$.

Main features:

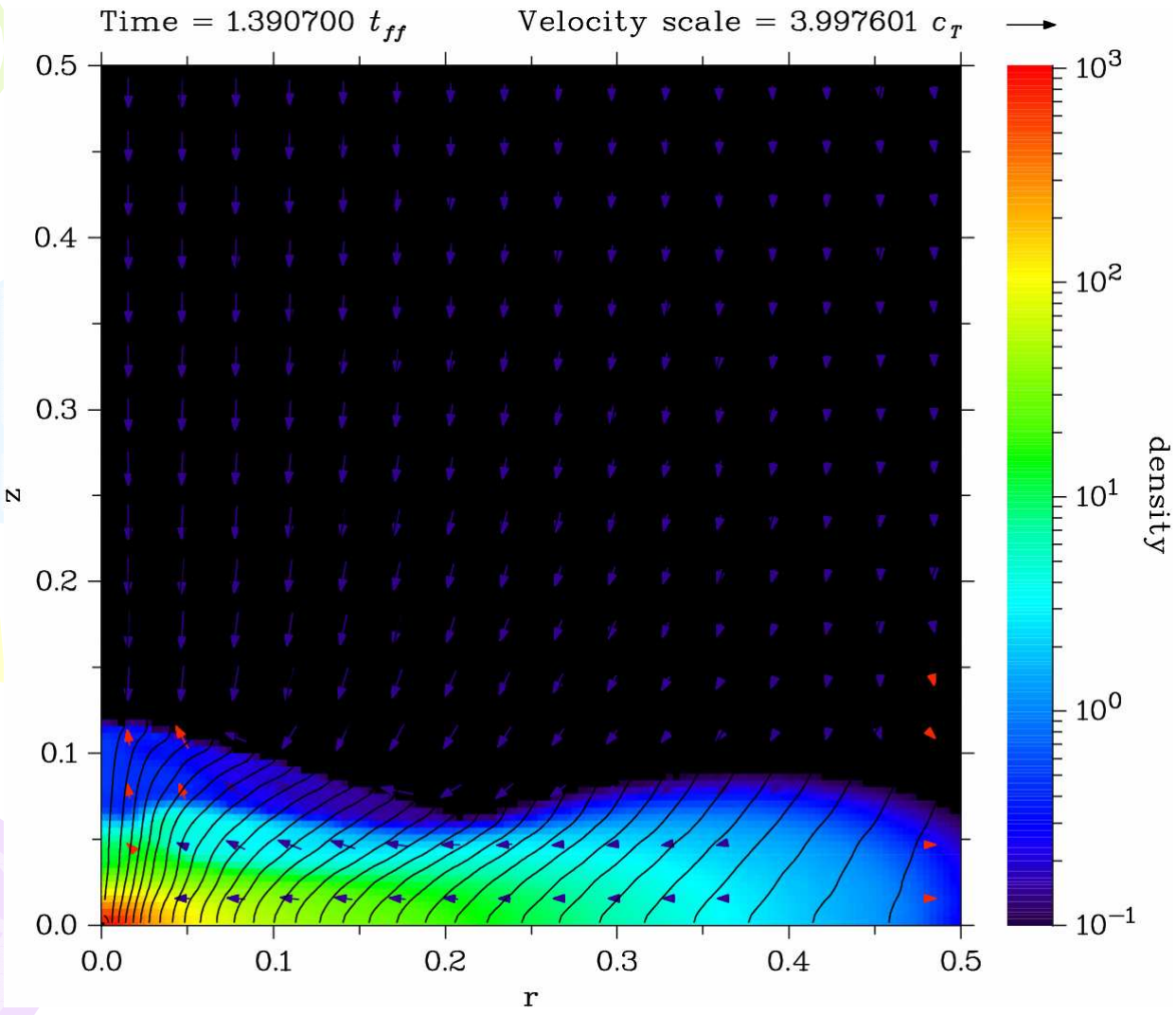
- Axial symmetry and spherical coordinates
- Accelerated Λ-iterations
- Long characteristics with Monte Carlo ray sampling
- Method for thermal balance calculations
- Linked with Leiden Molecular Database
- Various approximated methods are included
- Visualization tools: spectra maps, beam convolution..
- Tools for analysis

Ya. Pavlyuchenkov & B. Shustov, Astronomy Reports, v. 48, N4, pp. 348-359 (2004)

M. Hogerheijde, van der Tak, 2000

Example: collapse of the molecular core,

1. Results of 2D MHD simulations, Zhilkin et al. INASAN, Moscow



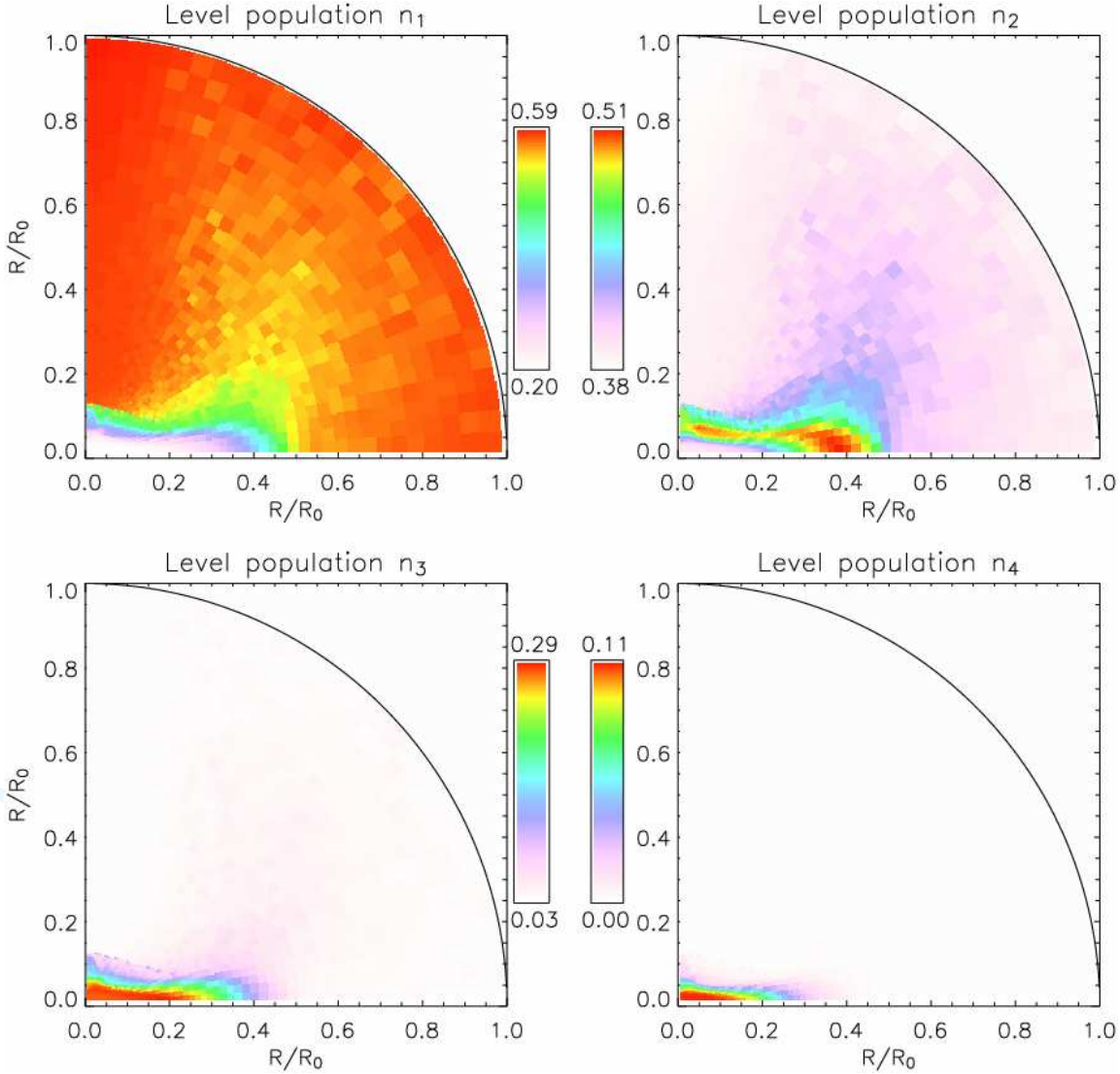
$M=5M_{\odot}$
T=10K

$E_{therm}/E_{grav}= 0.34$
$E_{rot}/E_{grav}= 0.2$
$E_{mag}/E_{grav}= 0.1$

$X(HCO^+)=5x10^{-10}$

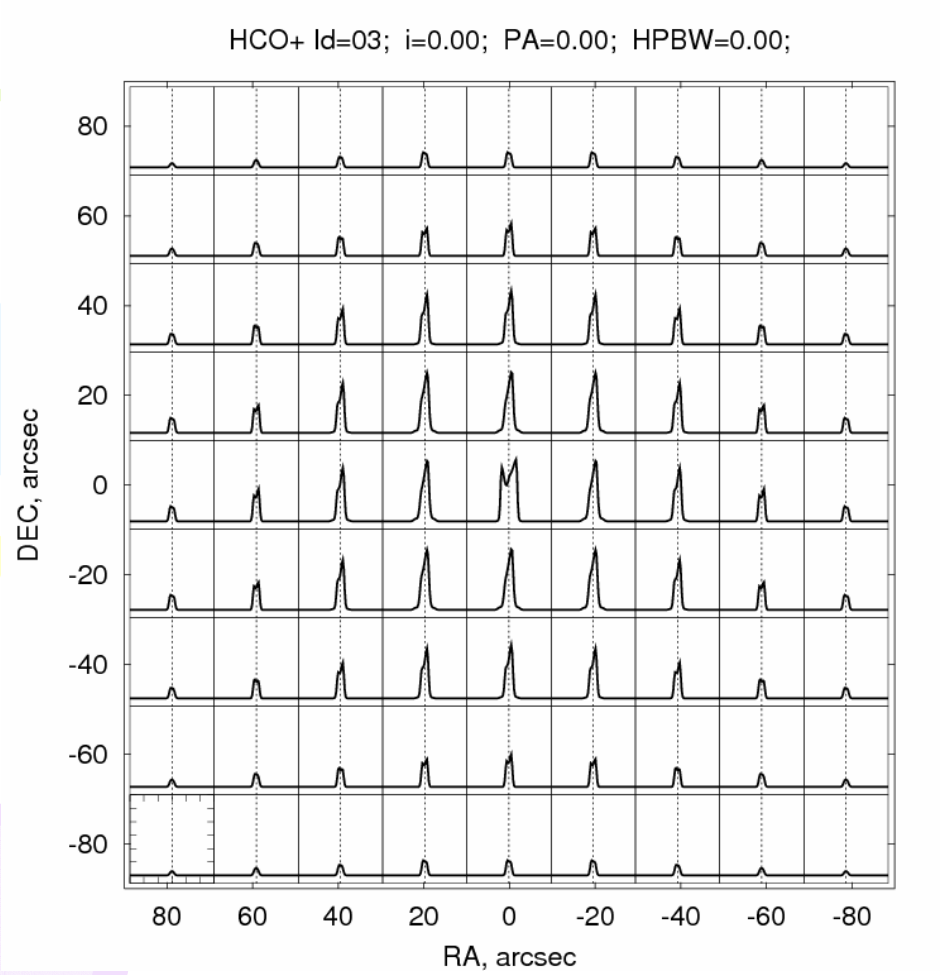
Example: collapse of the molecular core,

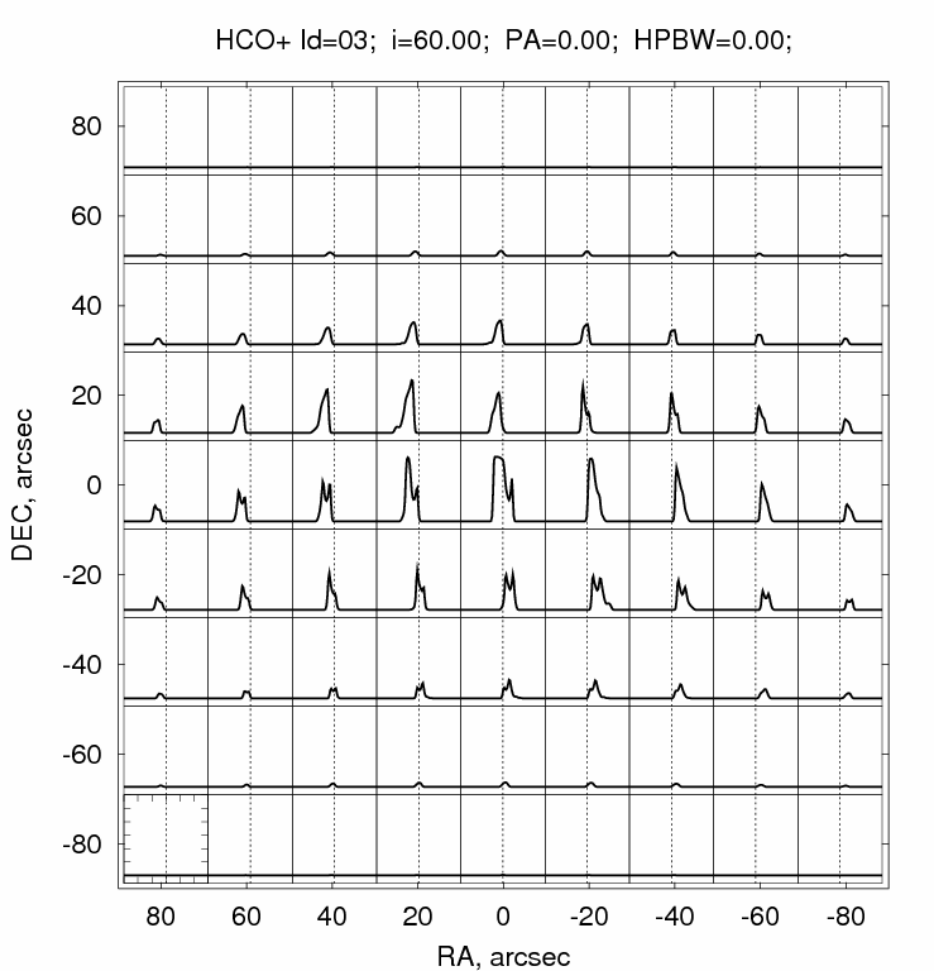
2. Results of LRT calculations: level populations



Example: collapse of the molecular core,

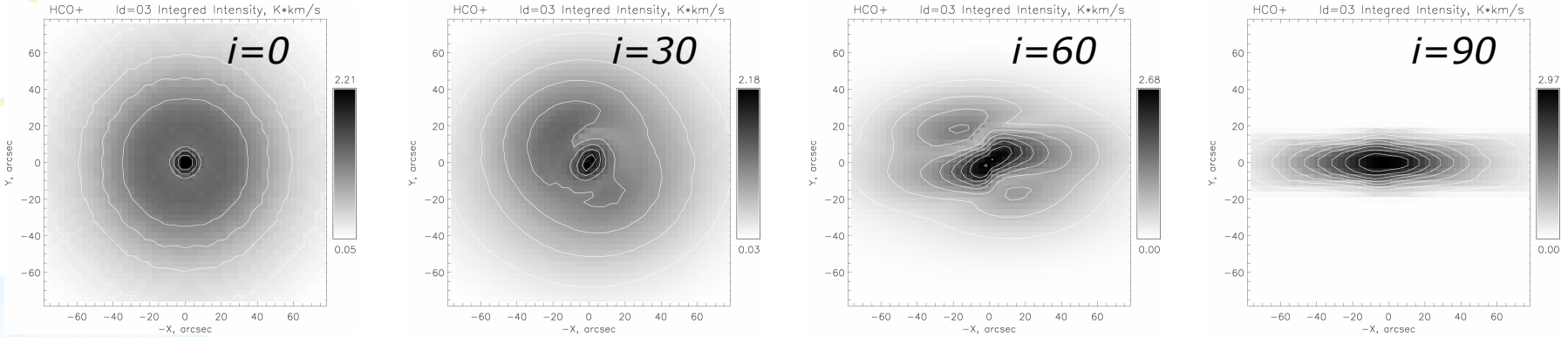
3. Results of LRT calculations: spectral maps for two spatial orientations of the model core



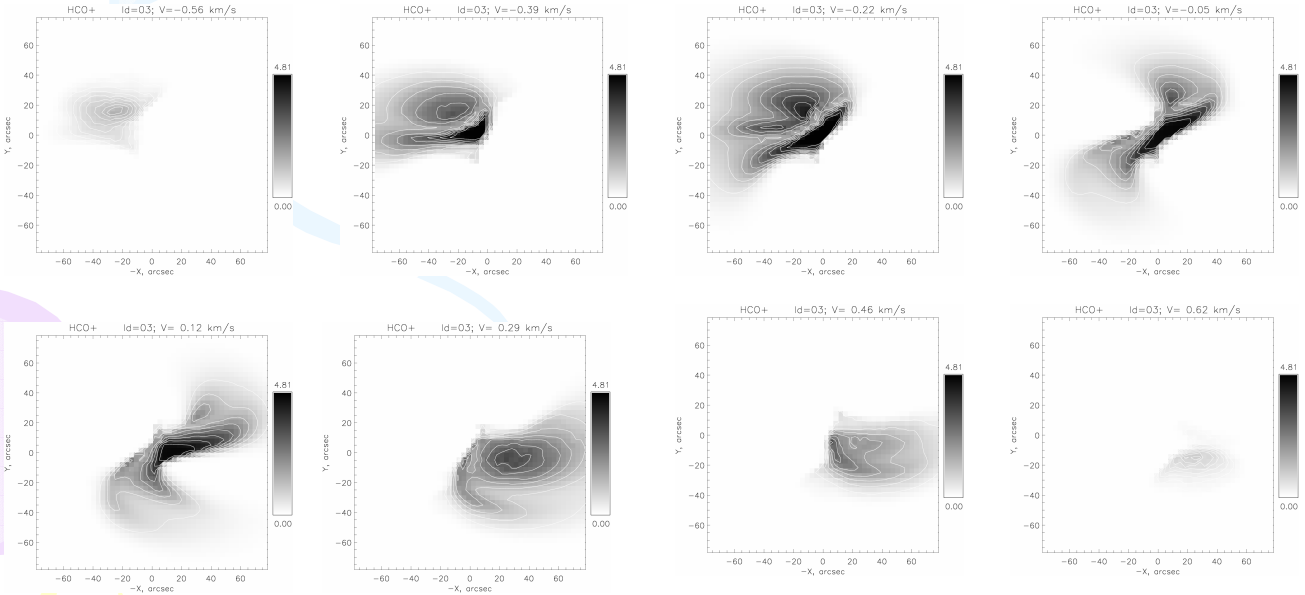


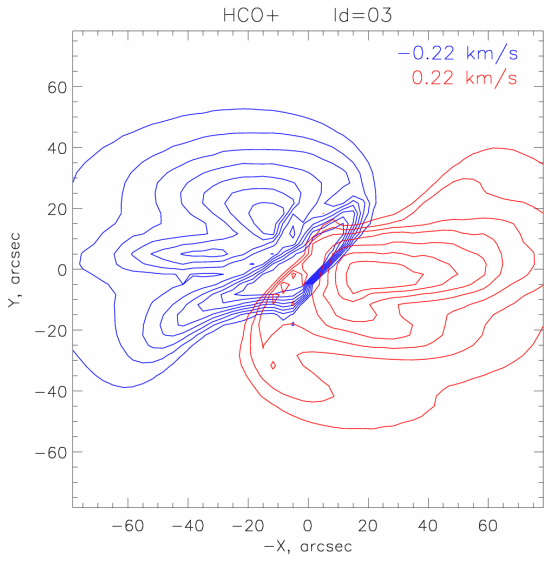
4. Results of LRT simulations: maps of integral intensity and channel intensity maps

Integral intensity maps for different inclinations



Channel intensity maps for different velocity offsets, *i=60*





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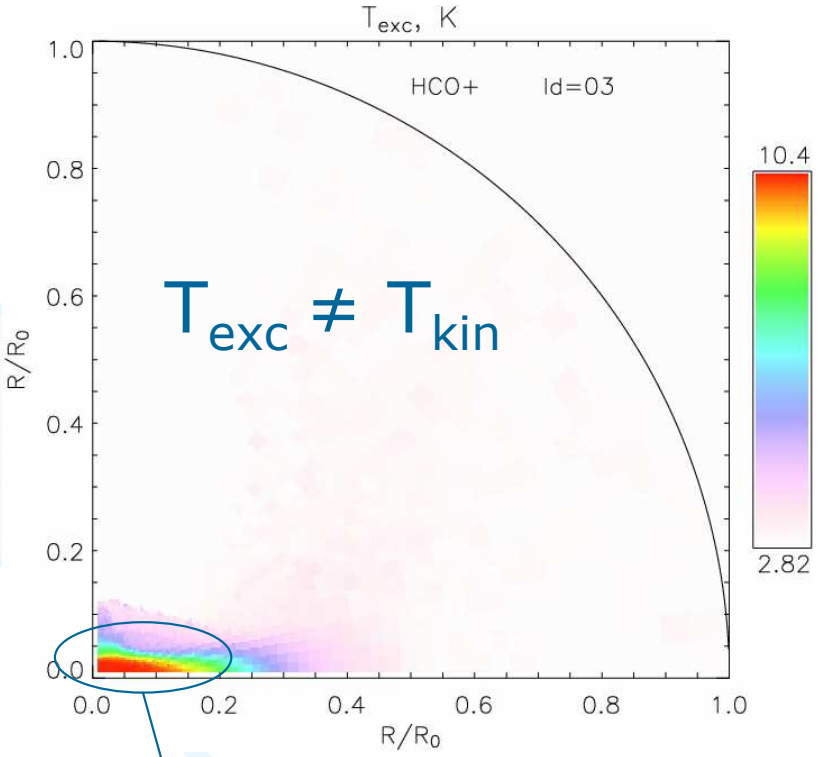
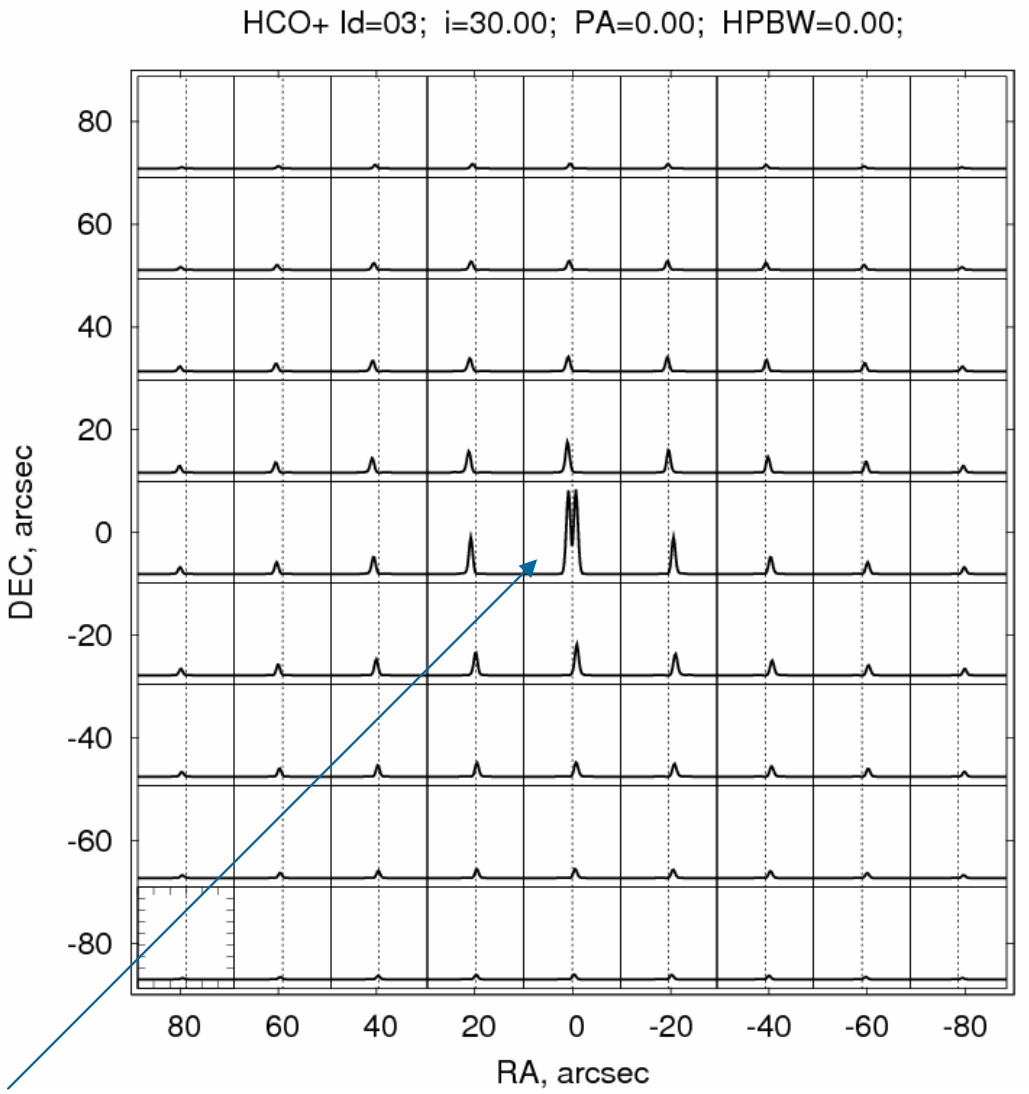
1. Distribution of excitation temperature and optical depth map



$T_{exc} \neq T_{kin}$

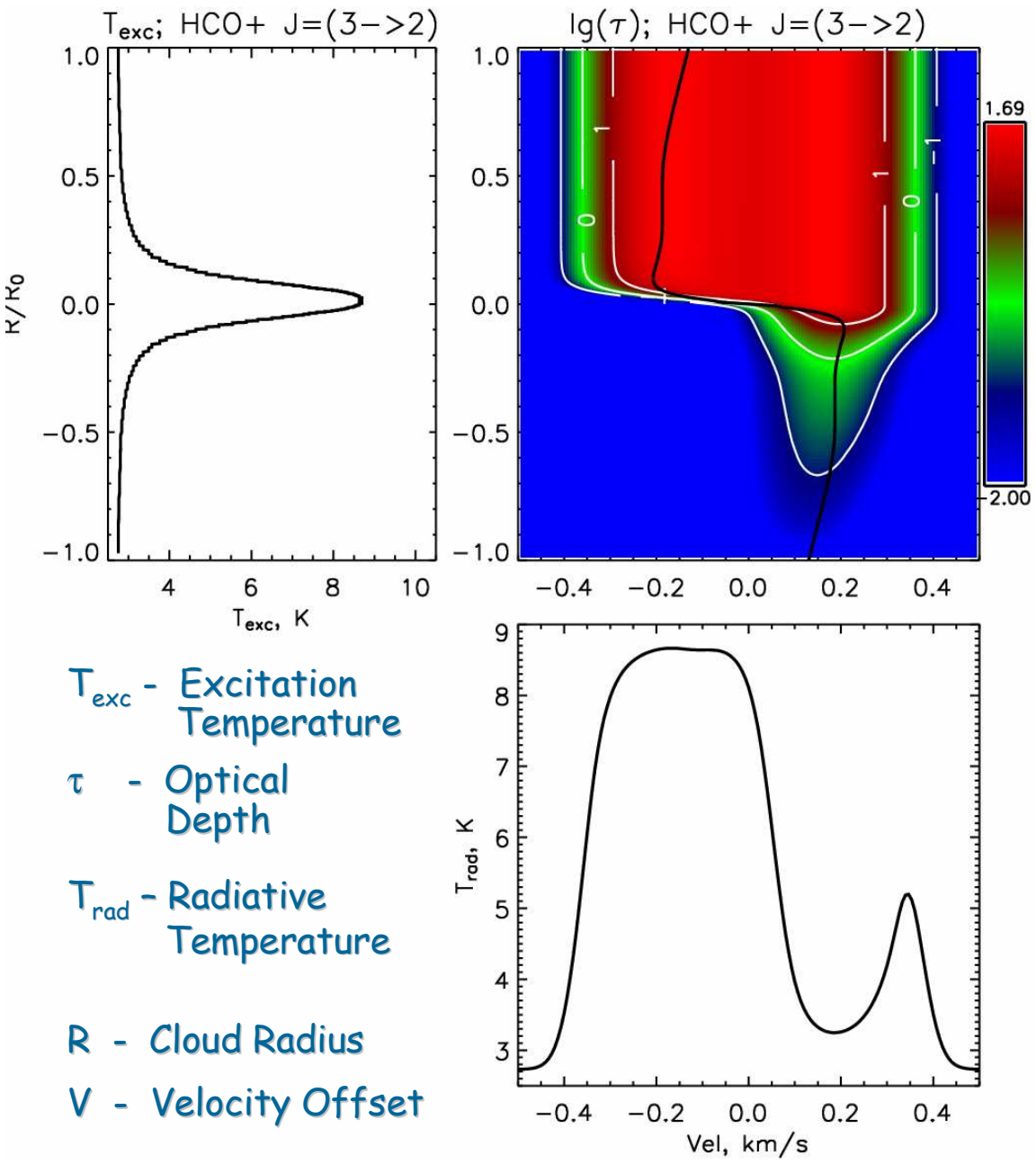
$T_{exc} = T_{kin}$



$\tau_{max} = 100$

2. Combined scheme of the molecular line formation

Formation of the HCO^+(3-2) profile for a model of prestellar core



T_{exc} - Excitation Temperature

τ - Optical Depth

T_{rad} - Radiative Temperature

R - Cloud Radius

V - Velocity Offset

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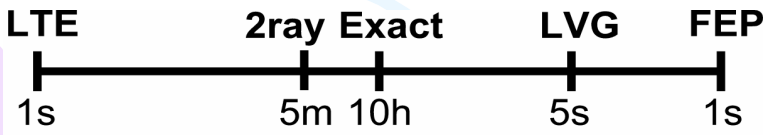
Multidimensional calculations may be too time consuming..

1. Approximated methods are available:

- LTE (local thermo-dynamical equilibrium)
- FEP (full escape probability approach)
- LVG (assumption of large velocity gradients)
- 2ray (assumption of marked directions)



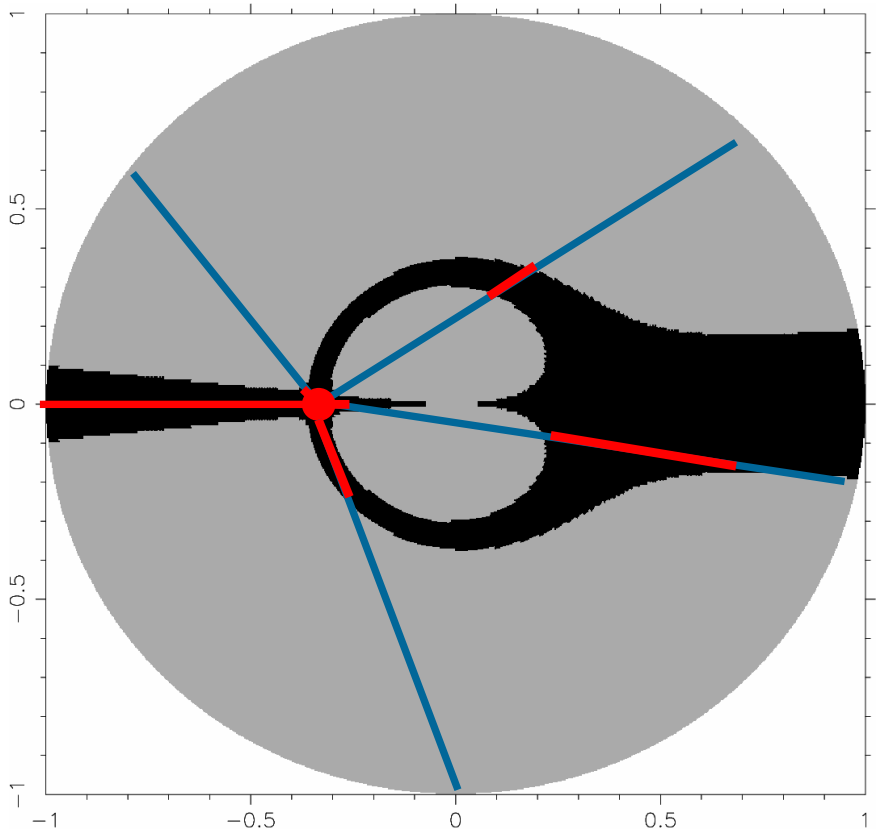
Typical computational demands of the LRT methods for protoplanetary disk simulations

2. Modifications to exact method:

- Concept of thermalized cells
- Concept of interacting cells

2. Concept of interacting cells. The case of Keplerian disk.

Black area represents the disk cells that are radiatively coupled to the red dot in the equatorial plane of the Keplerian disk ($V \propto r^{-0.5}$)



Allows to speed up the ray-tracing part of the code by a factor of >10 !

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Calculations of the thermal structure

Molecular lines affect the thermal structure of the prestellar objects. LRT simulations are necessary:

- to calculate gas temperature distribution
- to find the self consistent structure of the cloud
- to study importance of the thermo-chemical interaction

Molecular lines are not “tracers” any longer but important physical factor!

Example: the temperature of the diffuse cloud as a function of density:
(may be useful for HD simulations of the cluster formation ☺)

Heating:

Cosmic Rays,
Gas-Grains collisions,
Photoelectric Emission

Cooling:

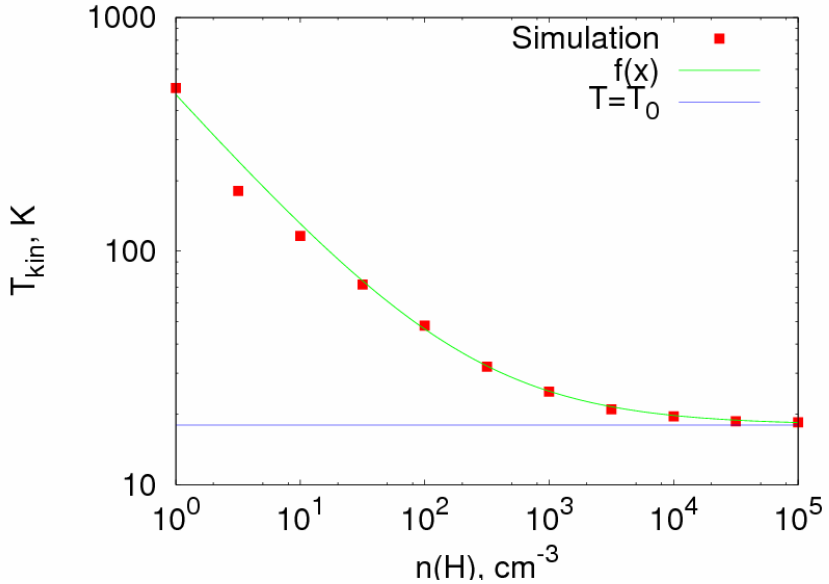
C^+ lines
Gas-Grains collisions

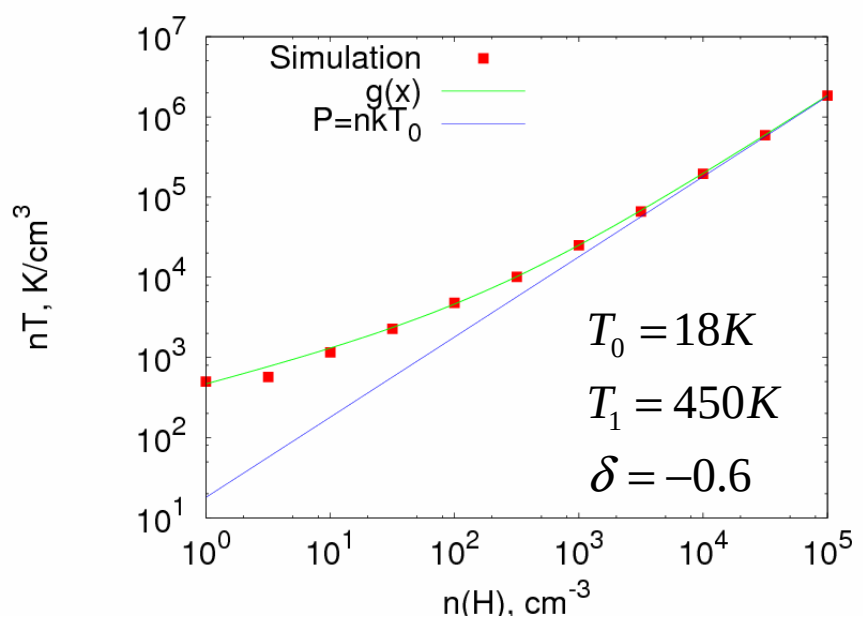
Results:

$$T(n) \approx T_0 + T_1 \left(\frac{n}{n_1} \right)^{\delta}$$

$$P \approx nkT_0 + \frac{kT_1}{n_1^{\delta}} n^{1+\delta}$$

isotherm polytrope





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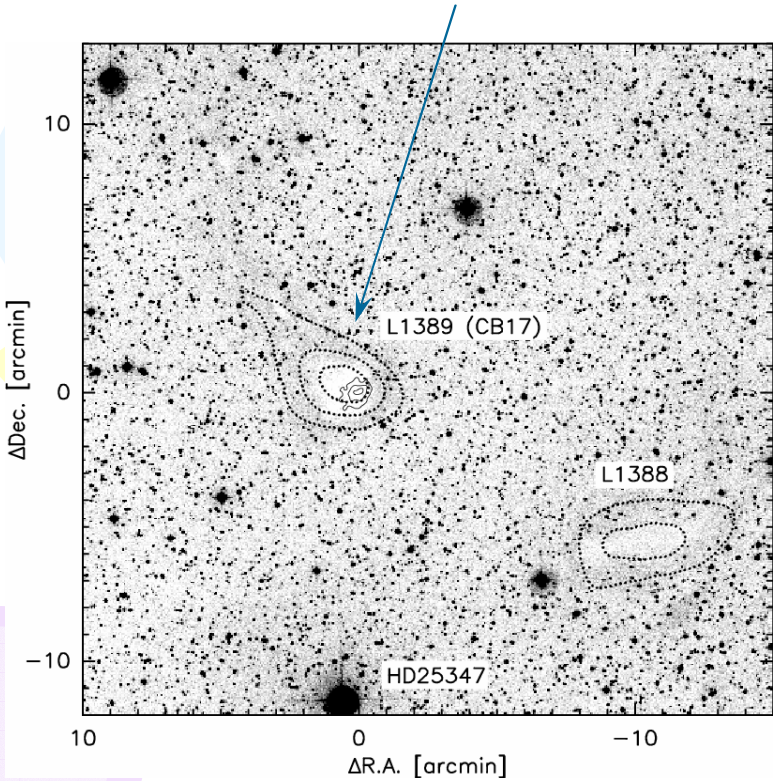
Observations of prestellar cores

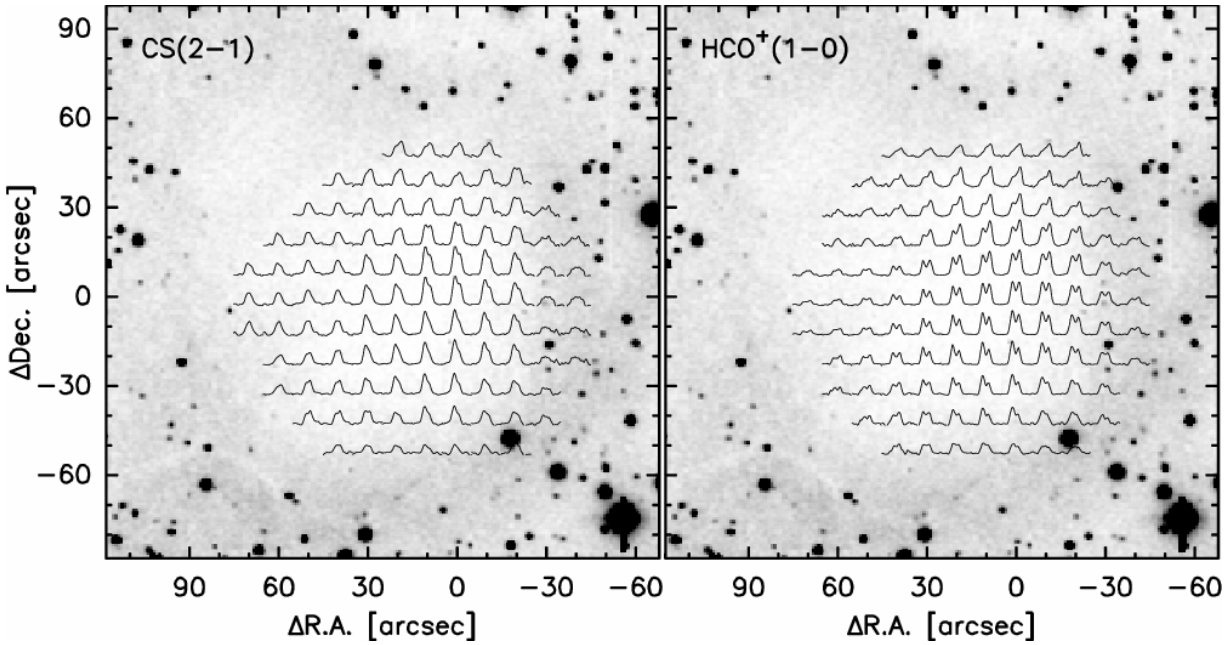
CB17 Bok globule is a relatively isolated low mass prestellar core

CB17 in visual



Map is taken from DSS2

CB17 in molecular lines

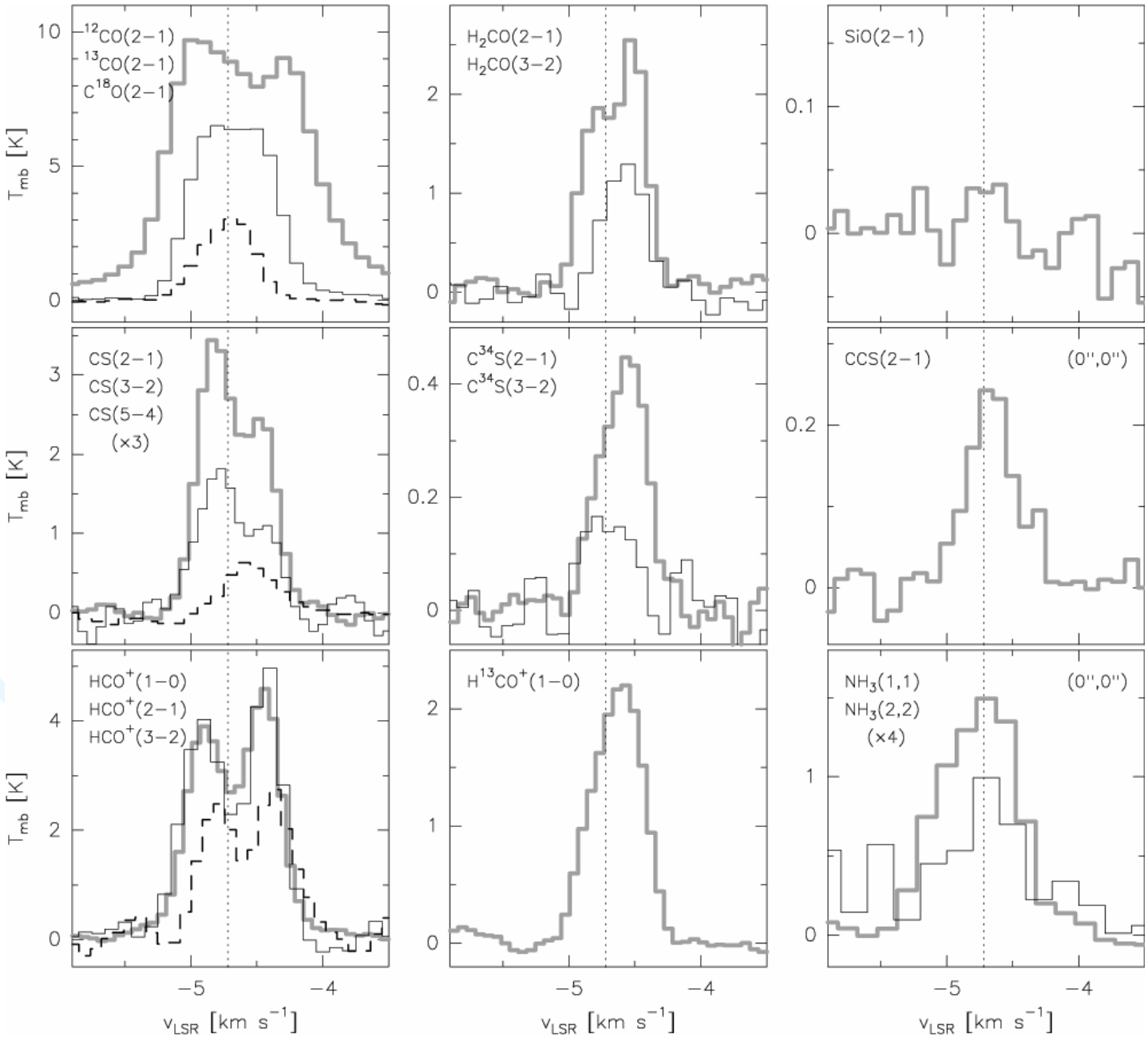


Maps are taken from Launhardt & Henning, in prep.

Table 1. Molecular line observations of CB 17

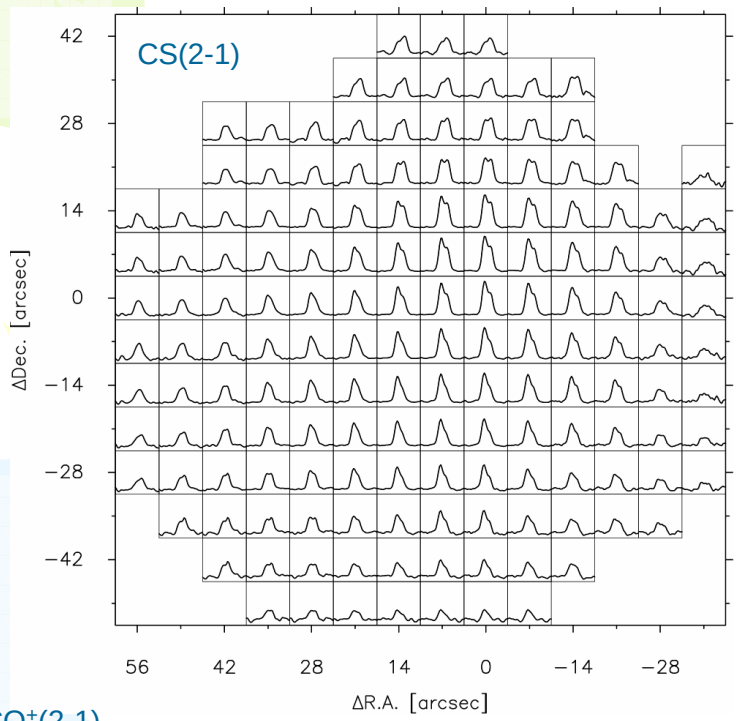
Line	Frequ. [GHz]	Telescope	Date [mo/yr]	HPBW [arcsec]	Δv [m s^{-1}]	$\eta_{\rm mb}$	Map size/ grid spacing
^{12}CO (2–1)	230.537990	IRAM 30m	10/96	10.4	130	0.45	105″/ 7″
^{13}CO (2–1)	220.398686	IRAM 30m	10/96	10.9	106	0.48	84″/ 7″
C^{18}O (2–1)	219.560319	IRAM 30m	10/96	10.9	107	0.48	35″/ 7″
CS (2–1)	97.9809680	IRAM 30m	06/93	25	60	0.76	80″/ 20″
CS (2–1)	97.9809680	IRAM 30m	10/96	25	60	0.73	91″/ 7″
C^{34}S (2–1)	96.4129820	IRAM 30m	06/93	25	81	0.76	2 pts
C^{34}S (2–1)	96.4129820	IRAM 30m	10/96	25	61	0.75	28″/ 7″
CS (3–2)	146.969049	IRAM 30m	06/93	17	80	0.68	80″/ 20″
C^{34}S (3–2)	144.617147	IRAM 30m	06/93	17	81	0.68	2 pts
CS (5–4)	244.935610	CSO 10.4m	01/96	30	58	0.70	30″/ 15″
CS(7–6)	342.882900	CSO 10.4m	01/96	24	52	0.65	1 pt
HCO$^+$ (1–0)	89.188523	IRAM 30m	10/96	27	66	0.82	112″/ 7″
H^{13}CO$^+$ (1–0)	86.7542884[a]	IRAM 30m	10/96	29	67	0.82	84″/ 7″
HCO$^+$ (2–1)	178.375047	IRAM 30m	10/96	14	66	0.56	112″/ 7″
HCO$^+$ (3–2)	267.557625	IRAM 30m	10/96	10	88	0.48	28″/ 7″
H_2CO 2(0,2)–1(0,1)	145.602952	IRAM 30m	10/96	17	80	0.60	28″/ 14″
H_2CO 3(0,3)–2(0,2)	218.222188	IRAM 30m	10/96	10.9	107	0.48	28″/ 14″
SiO (2–1,ν=0)	86.846981	IRAM 30m	10/96	29	67	0.82	28″/ 7″
CCS (2_1–1_0)	22.344033	Eff. 100m	03/99	41	82	... [b]	1 pt
NH_3 (1,1)	23.6944965	Eff. 100m	03/99	41	154	... [b]	1 pt
NH_3 (2,2)	23.7226315	Eff. 100m	03/99	41	154	... [b]	1 pt

Line profiles toward the center

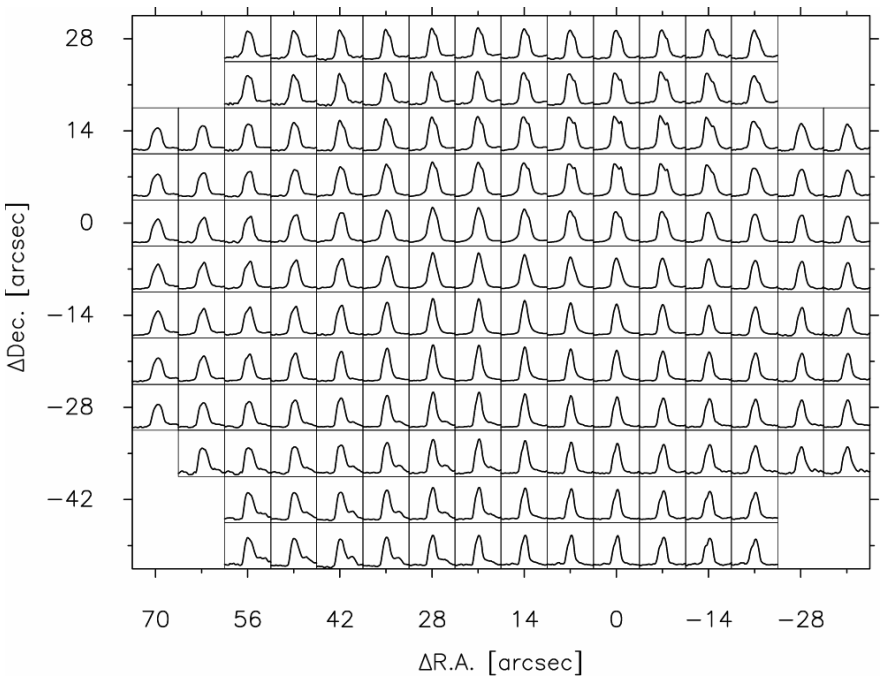


Some of spectra maps for CB17

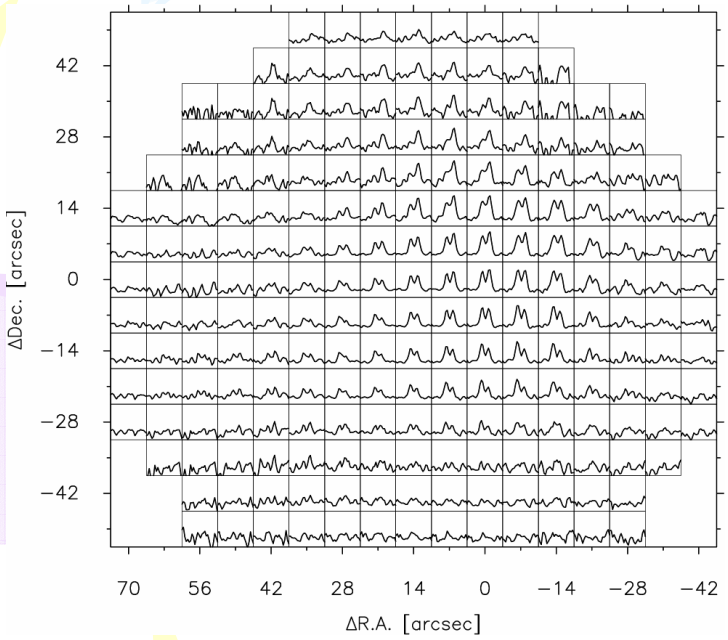
CS(2-1)



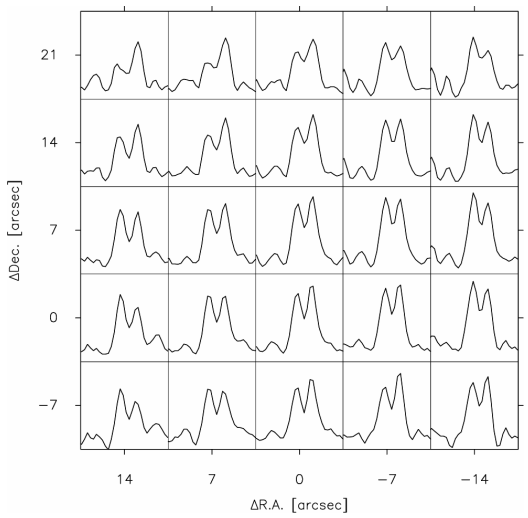
CO (2-1)



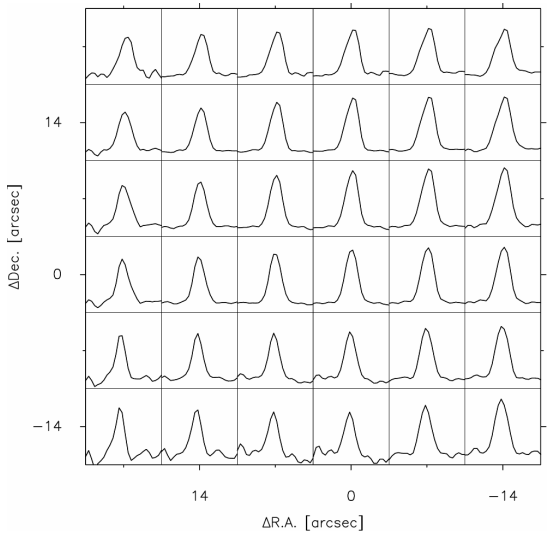
HCO^+(2-1)



HCO^+ (3-2)



$C^{18}O$(2-1)



Main parameters of the CB17 core:

Mass: $M = 6M_{\odot}$

Temperature: $T = 10$ K

Radius: $R = 2.3 \cdot 10^4$ AU

Density distribution:

$$n(H_2) = \frac{n_0}{1 + (r/r_0)^p}$$

$n_0 = 7 \cdot 10^5$ cm^{-3}
$r_0 = 3000$ AU
$p = 2.2$

Distance: D = 300 pc

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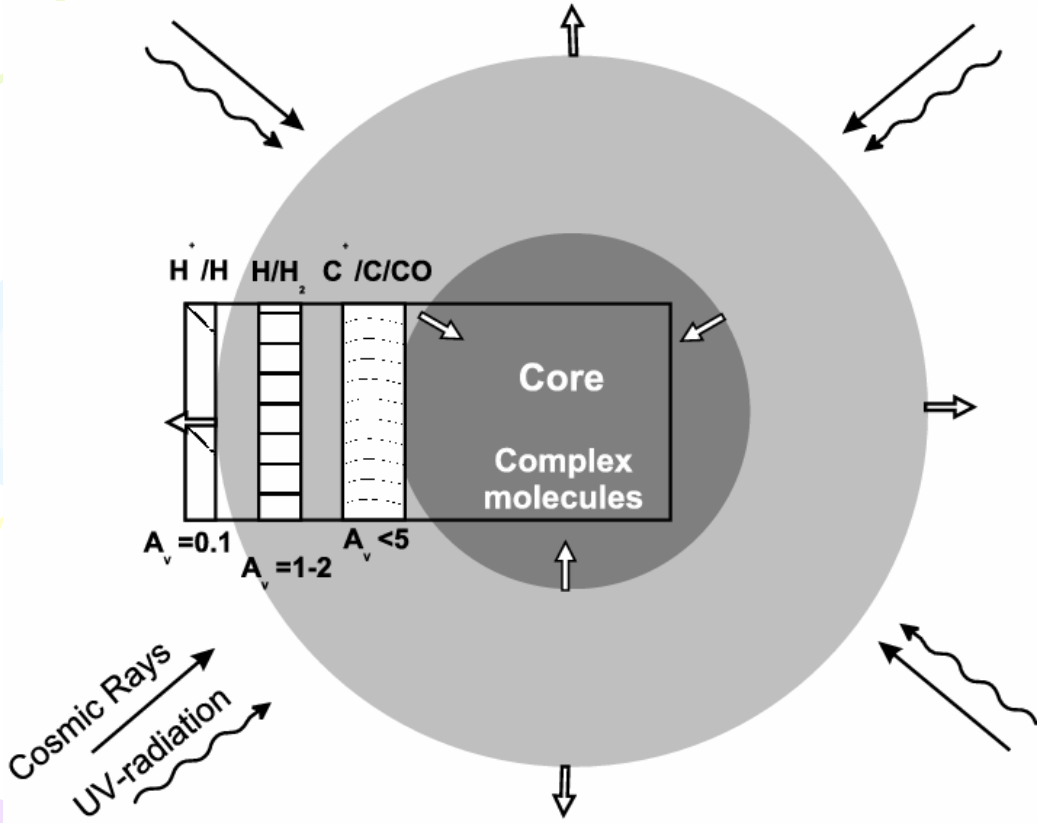
Outline of the prestellar core structure



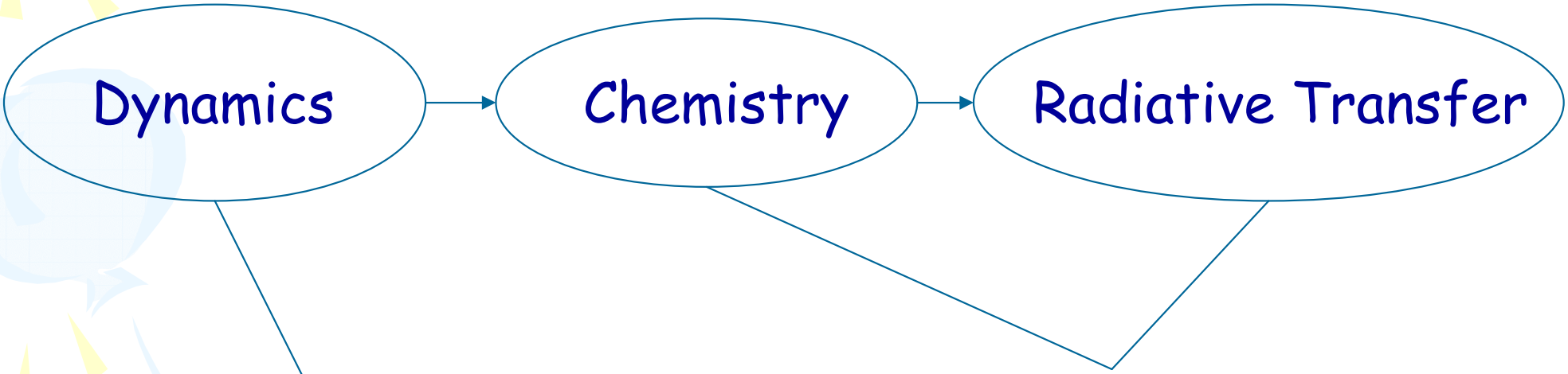
Molecular lines affected by:

- Density structure
- Thermal structure
- Kinematical structure
- Chemical structure

Chemical structure affected by:

- Density and thermal structure and their evolution with time
- External UV field
- Cosmic ray intensity
- Depletion onto dust grains

What are the most important factors which should be taken into account when we deal with molecular line profiles of prestellar cores?



We focus on these two steps to study related factors!

Using some prescription of the core dynamics

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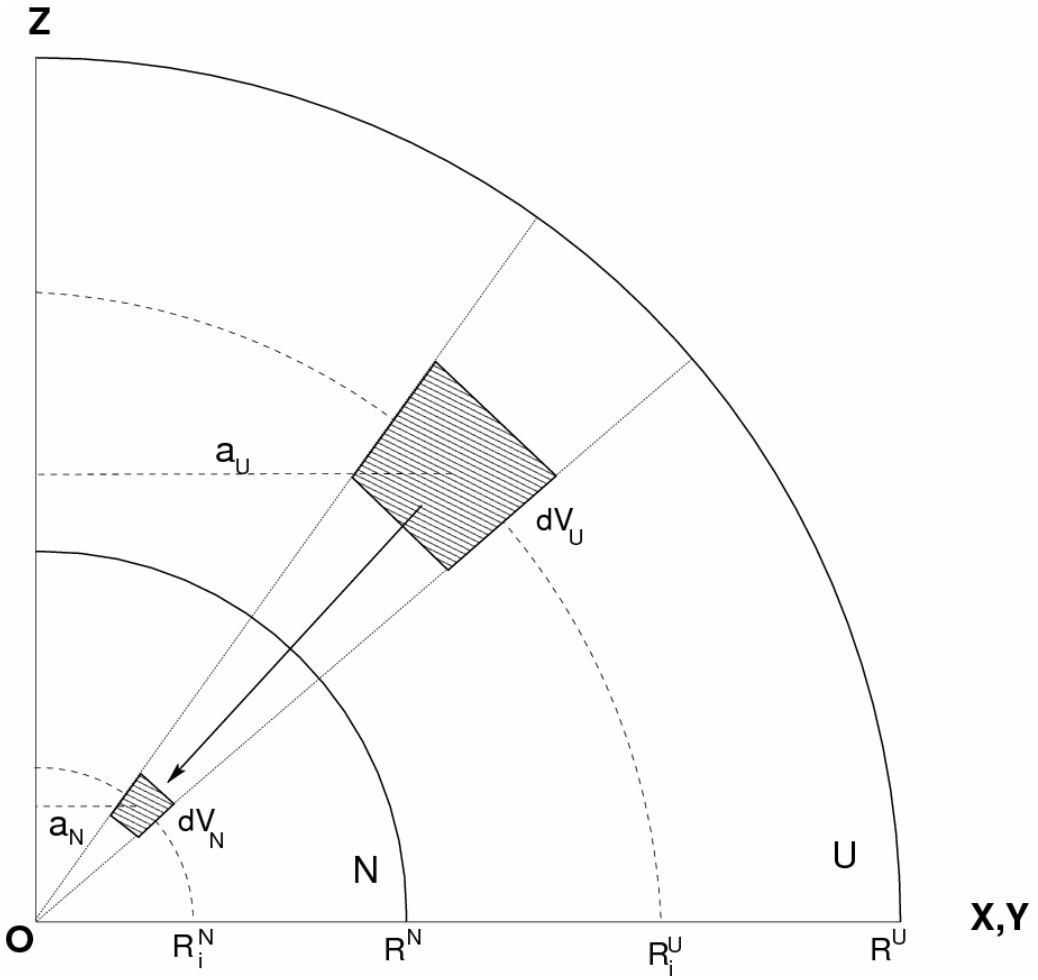
Kinematical model: phenomenological prescription

1. Initial and final density configuration
2. Postulated law of contraction
3. Angular momentum conservation



$$R_i(t) = R_i(0) - W_i\left(\frac{t}{t_0}\right)^{\delta},$$

$$V_i(t_0) = -\delta\frac{W_i}{t_0}$$

Evolution time, t_0

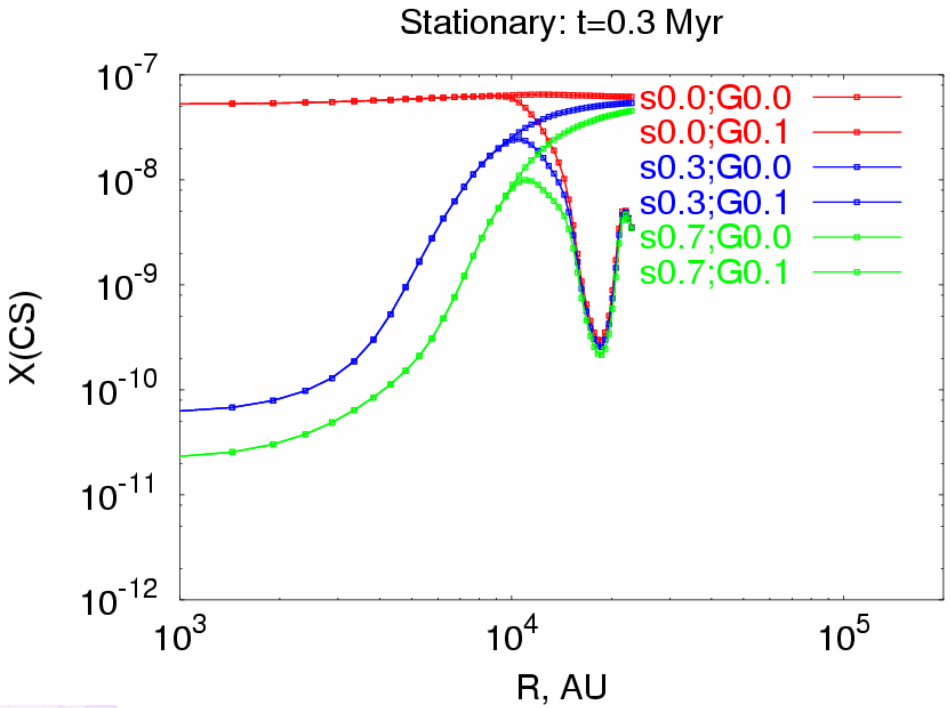
Power law index, δ

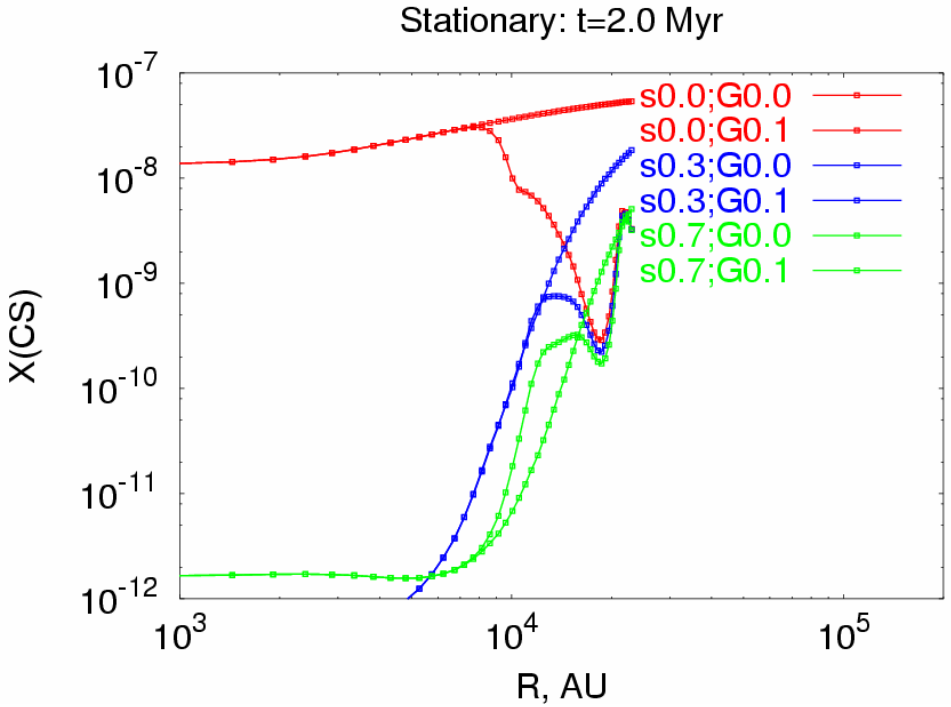
Initial angular velocity, Ω_0

Chemical model: Semenov et al. A&A, 2004, Wiebe et al. A&A, 2003

Crucial parameters:

- Sticking probability, S
- Intensity of UV field, G
- Cosmic ray intensity, CR





Distributions of CS abundances for the static models with following parameters: t=0.3; 2.0 Myr; G=0.0; 0.1G_0, S=0.0; 0.3

1. Introduction to LRT numerical simulations

- Concept of the LRT simulations
- In-depth analysis of the LRT simulations
- Improved and approximated methods
- Calculation of the thermal structure

2. LRT simulations of prestellar cores

- Observations of prestellar core
- Goals of phenomenological models
- Scheme of the model
- Parameter study of CB17

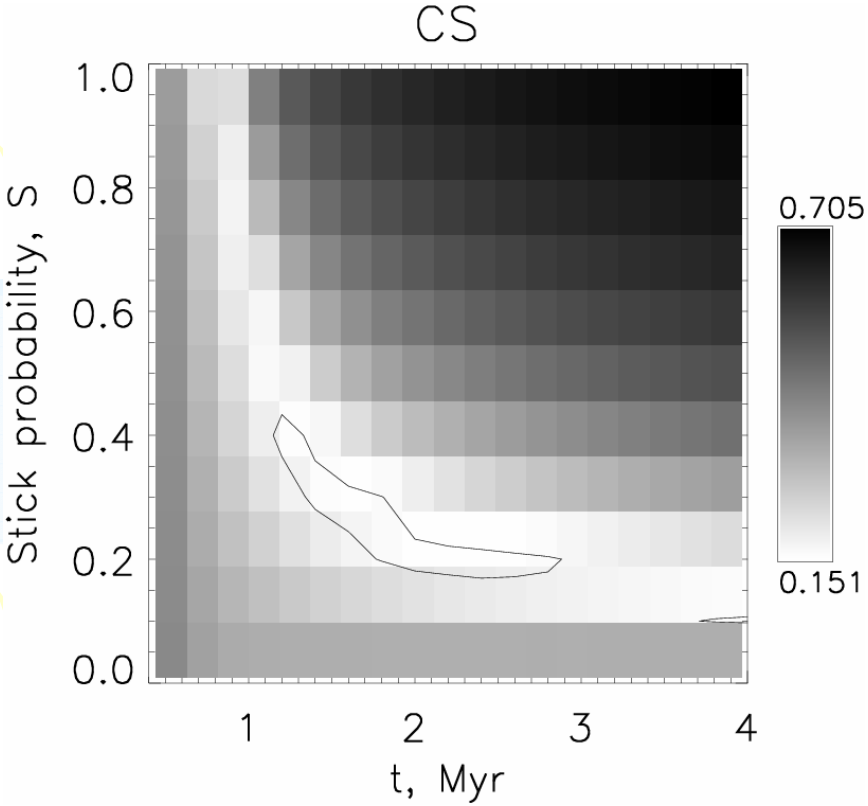
Multidimensional parameter search for:

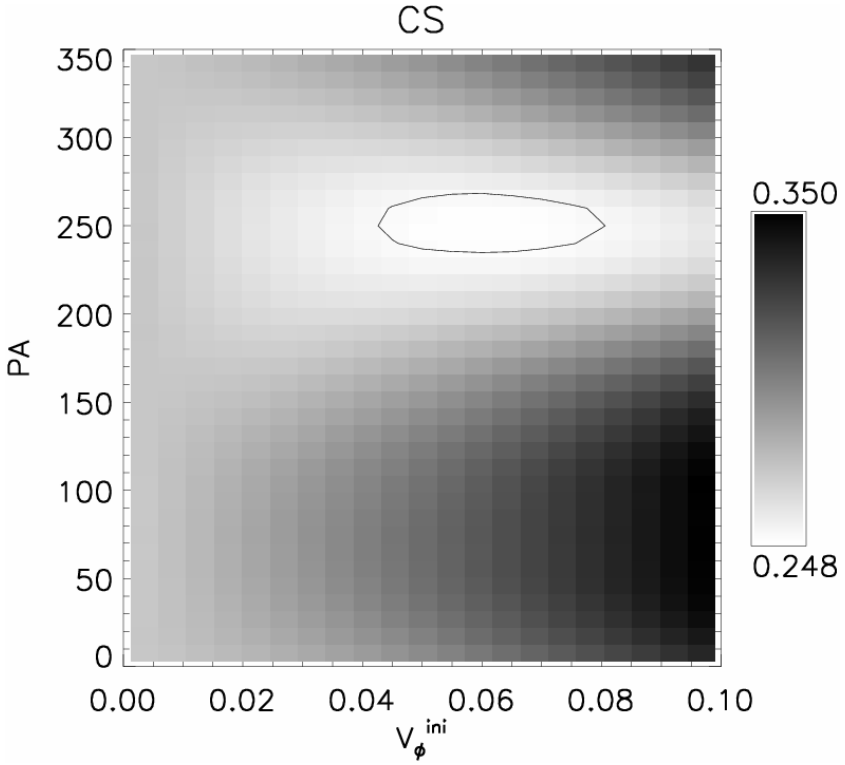
- Evolution law: t_0, δ
- Sticking probability, S
- UV strength, G
- Angular velocity, Ω
- Spatial orientation, PA

Each of ~1000 models includes:

- Simulation of chemical evolution on the top of dynamics
- Calculation of the molecular line profiles
- Evaluation of the agreement between calculated and observed line profiles

Agreement between calculated and observed maps for various model parameters





Criterion of the spectra fit:

$$SP = \frac{1}{J_{obs} + J_{model}} \sum \left| I_{obs} - I_{model} \right| \Delta V,$$

Outcome of the simulations:

- Infall velocity: V_r=50m/s
  Too small for free collapse?

- Rotation velocity: V_φ=100m/s
  Affects all the spectra maps

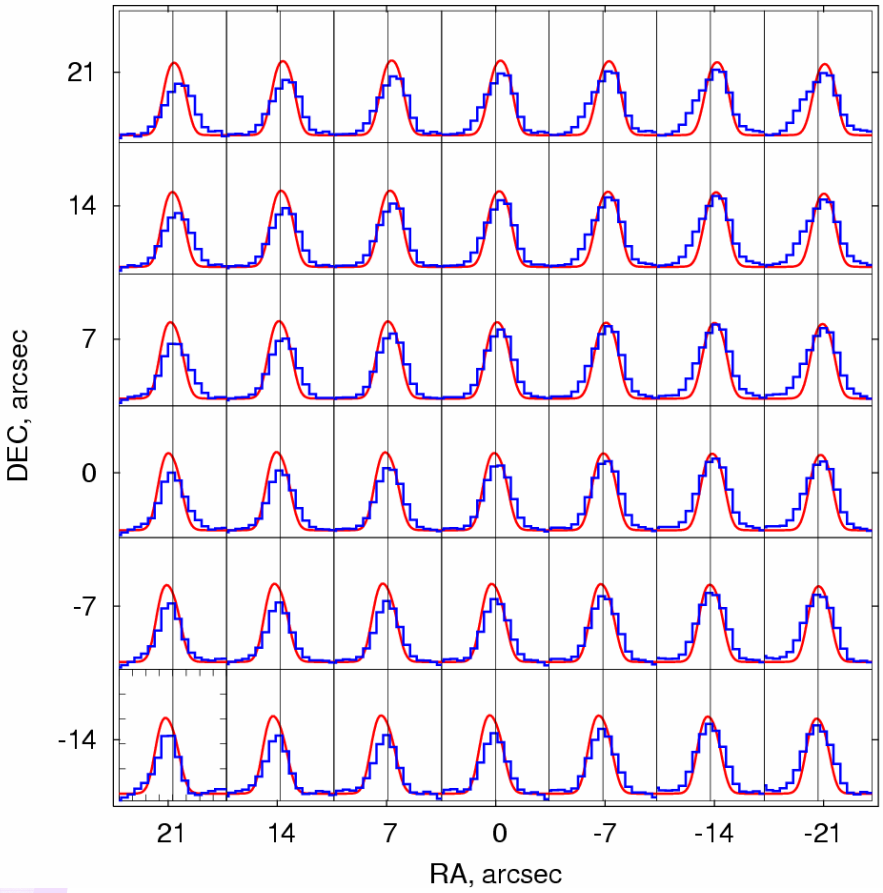
- Angular momentum: $J=1.6\times10^{21}$ cm^2/c
  Too large for the single star!

- Intensity of UV-field: 0.1 G_0
  Is crucial for the line features!

- Chemo-dynamical age: 2 Myr
  Sufficiently larger than freefall time?

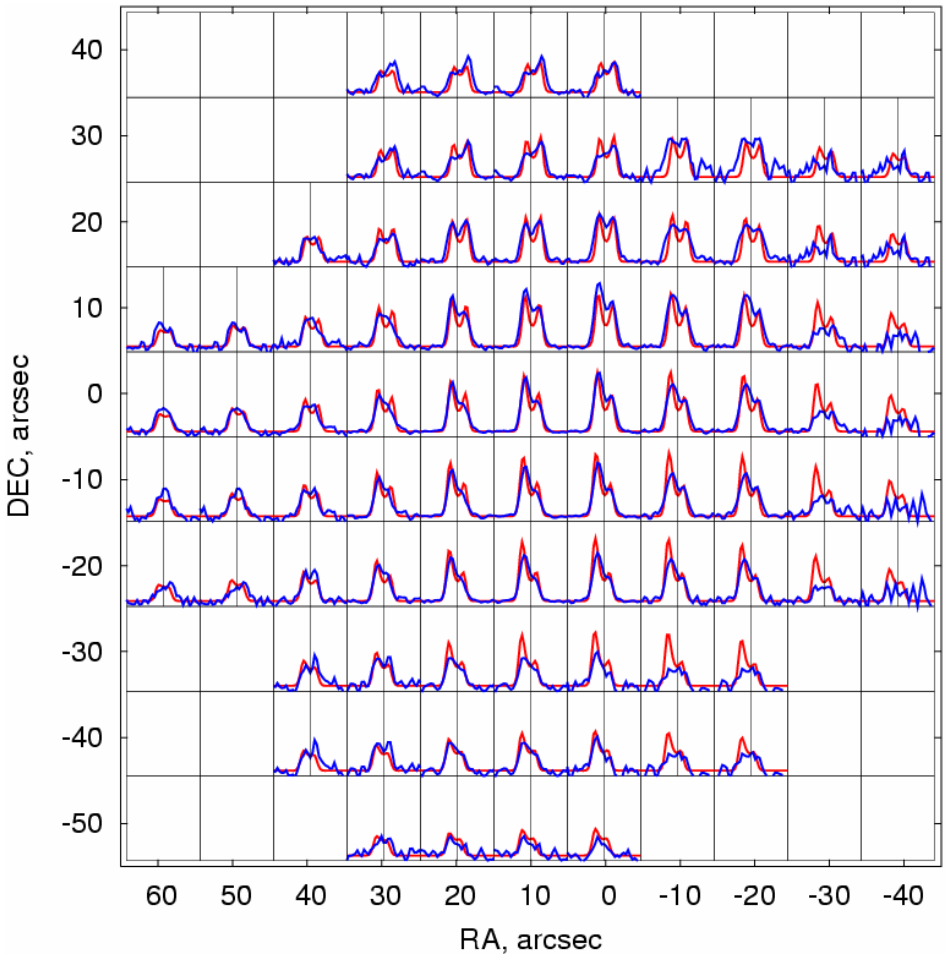
Observed and calculated spectra maps for best fit model

Observed and Modeled
line profiles of $C^{18}O(2\text{-}1)$



Optically thin lines

Observed and Modeled
line profiles of CS(2-1)



Optically thick lines

How reliable are these parameters?

There is a number of uninvestigated but very important factors:

- Uncertainties of cosmic ray intensity
- Chemistry on dust grains
- Initial state of the cloud
- Initial chemical content of the cloud
- Uncertainties of chemical rates

Let’s collaborate to answer these questions! ☺

Conclusions:

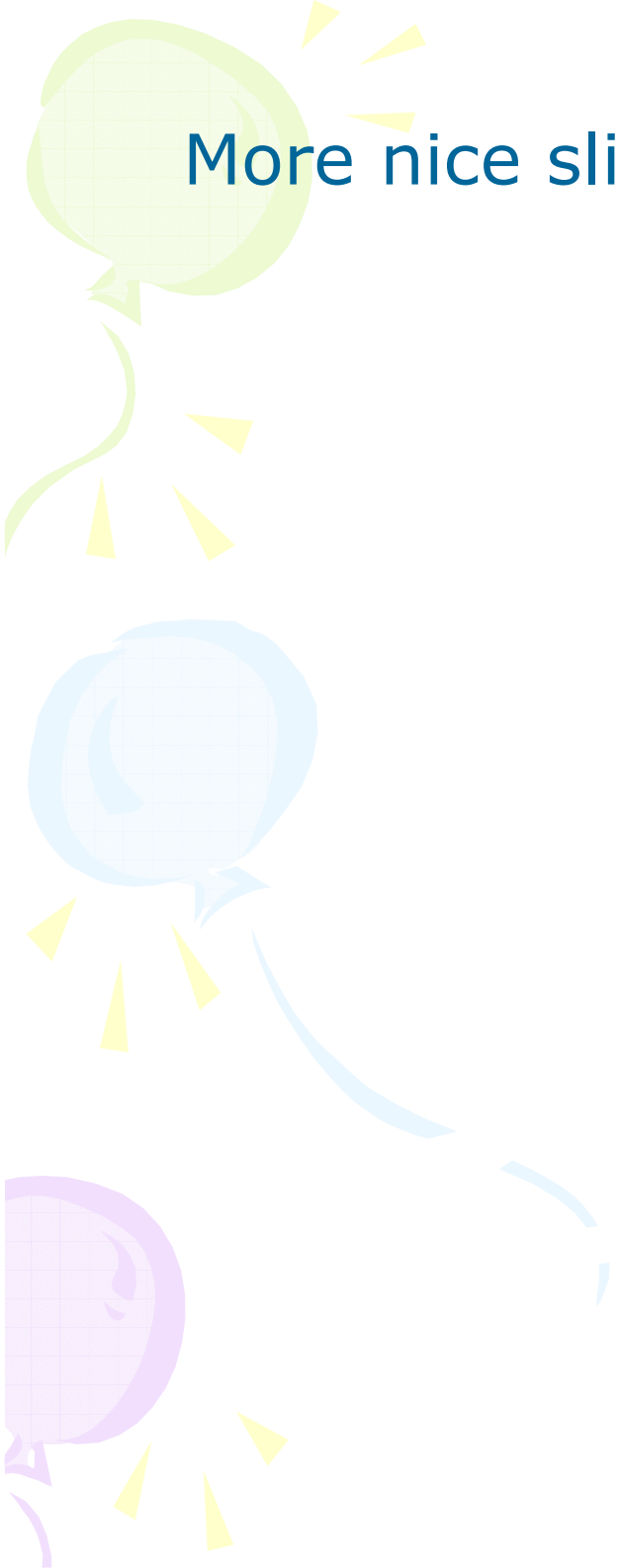
- Molecular line observations is valuable source of information about the physical and chemical structure and evolutionary status of the prestellar objects in general, and of the molecular cores in particular

- To derive this information we need to develop the self-consistent models coupled with LRT simulations

- For the many cases it is possible to use approximated and/or improved LRT methods which sufficiently speed up the computation time

- Given the sufficient number of the observed molecular lines it is possible to derive all the main parameters of the prestellar cores

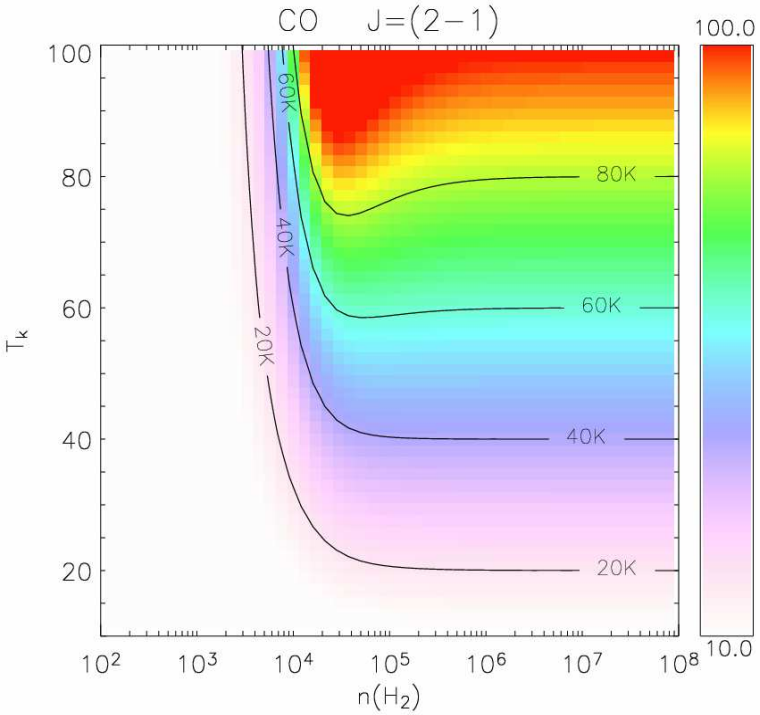
More nice slides ☺



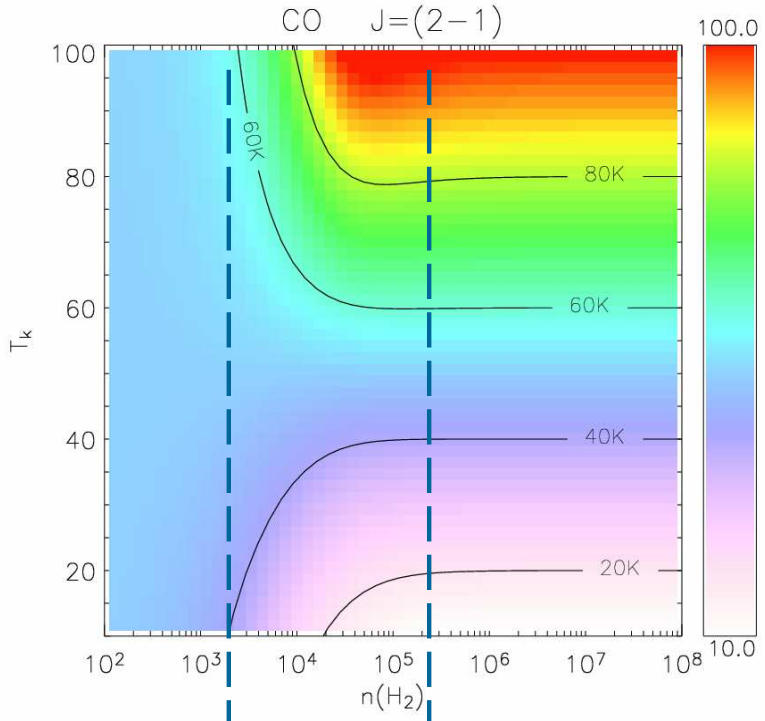
Excitation temperature maps

Molecule: CO

T_{bg}= 2.73 K



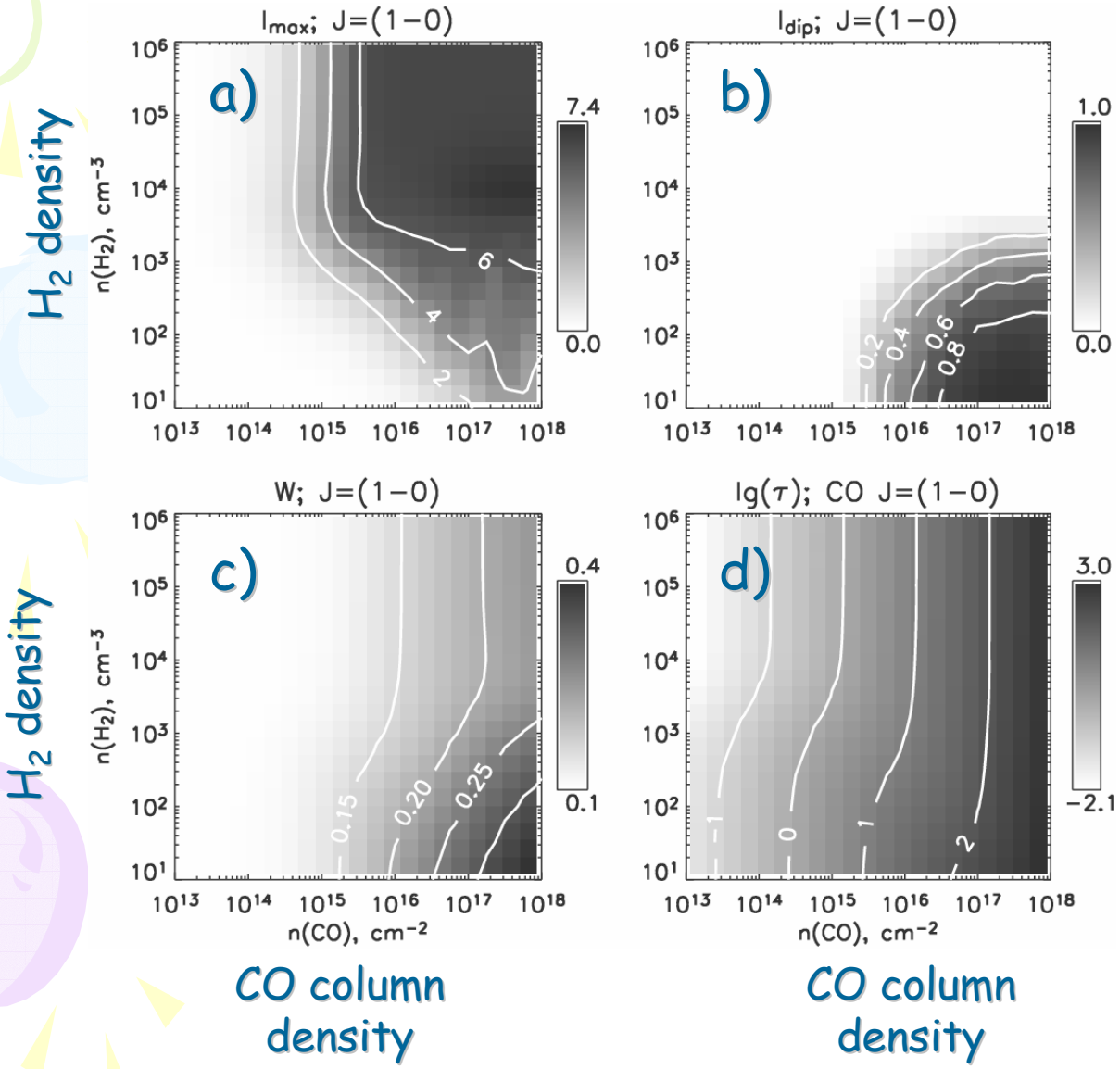
T_{bg}= 50 K



I II III

three zones!

General Theoretical Study of molecular line profiles



a) Max. Intensity,

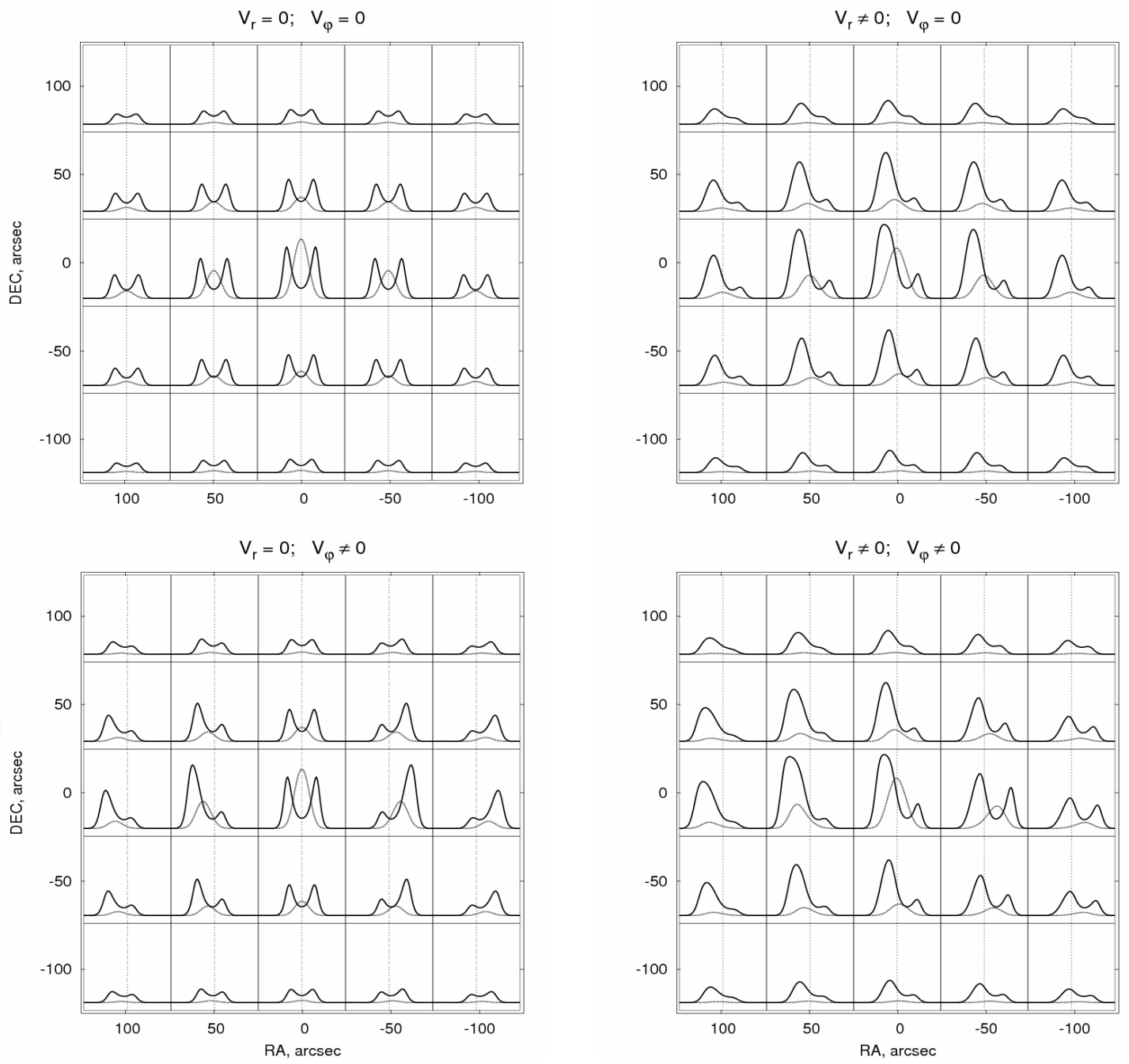
b) Strength of Self-absorption Dip,

c) Line Width, and

d) Max. Optical Depth

as a function of cloud parameters

Spectra maps for different cloud kinematics



Example: the temperature distribution in prestellar core (hydrostatic model + chemistry + continuum RT)

Heating:

Cosmic Rays,
Gas-Grains collisions,
Photoelectric Emission

Cooling:

Molecular Lines
Gas-Grains collisions

Parameters:

External field
Central Density
Chemical Age