

(THEORY OF)

# RADIATIVE TRANSFER AND MOLECULAR EXCITATION

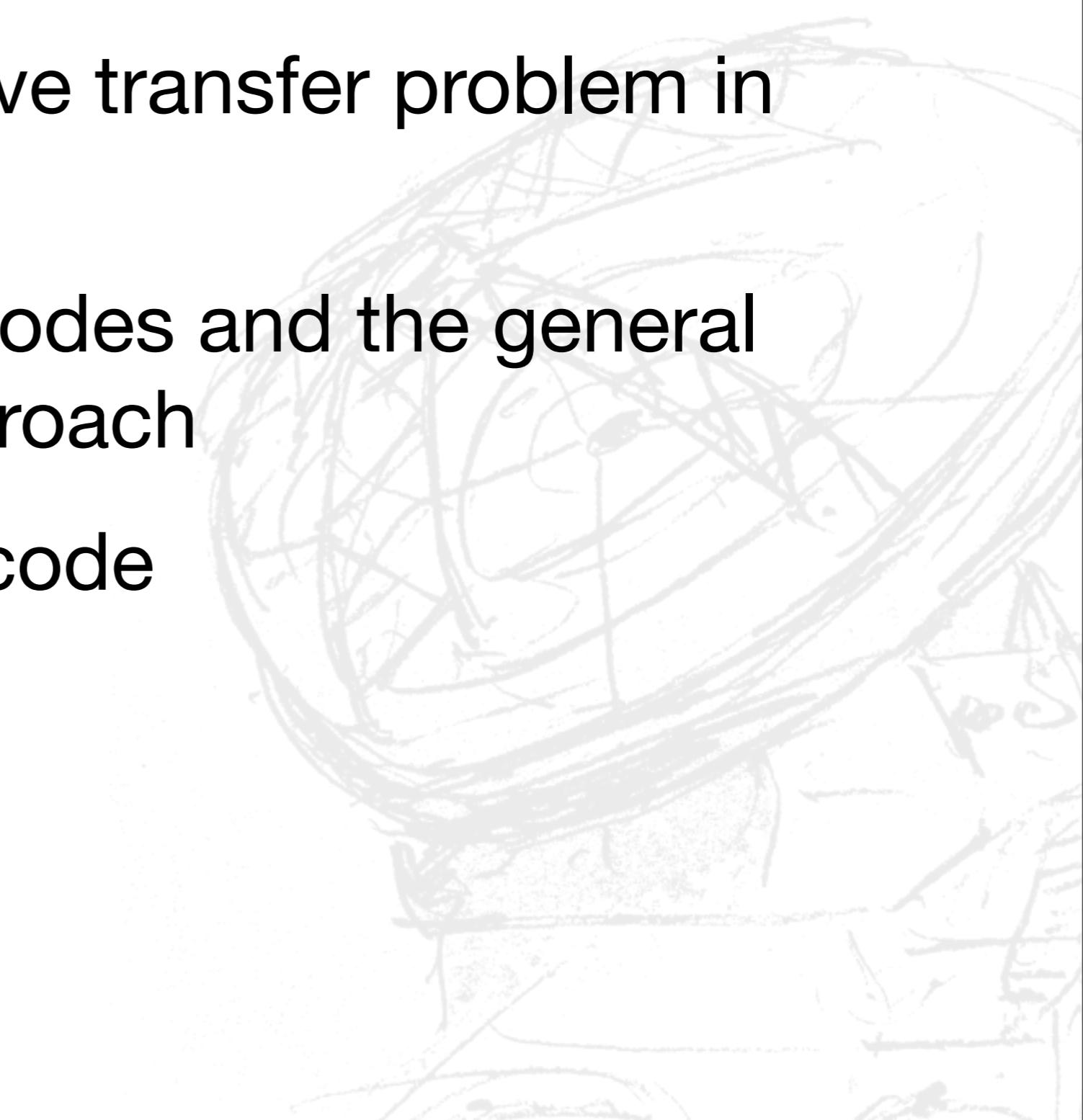


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University of Copenhagen

Leiden, February 28, 2012

# OUTLINE

- The radiative transfer problem in astronomy
- Available codes and the general model approach
- The LIME code
- Examples

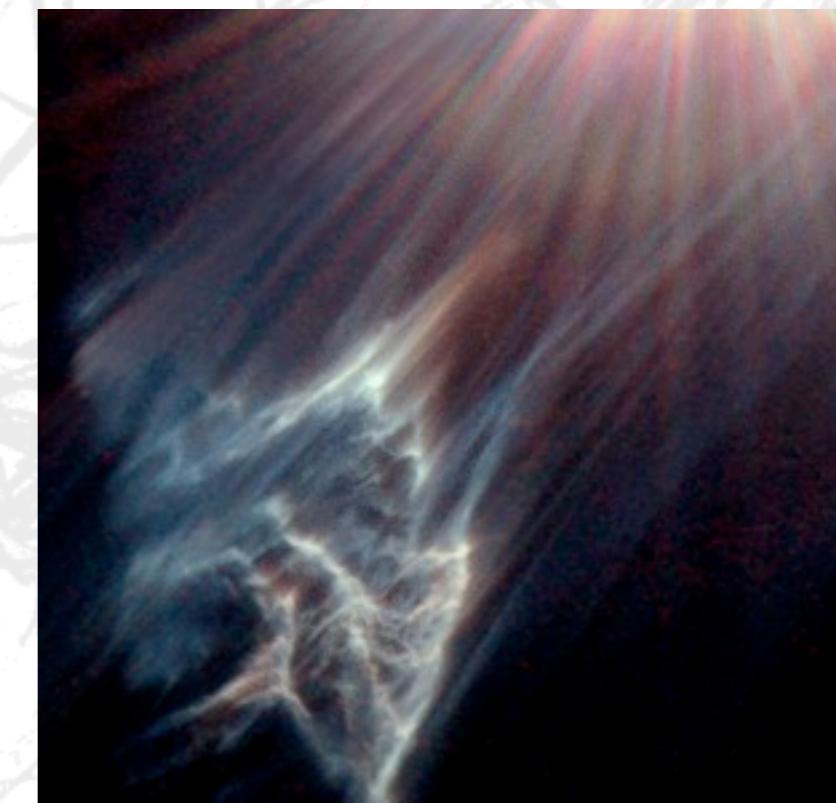


RT is important for  
astronomy

also atmospheric  
research, remote sensing,  
medical imaging, and  
nuclear weapons

# DEFINITION

Radiative transfer theory describes the propagation of light in a medium and its interaction with matter through emission, absorption, and scattering processes.



Inhomogeneous first-order linear constant coefficient ordinary differential equation

# EQUATION OF RADIATIVE TRANSFER

$$\frac{dI_\nu}{d\tau_\nu} = I_\nu - S(\tau_\nu)$$

$$\tau_\nu = \int \alpha_\nu ds$$

$$S \equiv j_\nu / \alpha_\nu (+\sigma_\nu / \alpha_\nu)$$

$j_\nu$  emission coefficient

$\alpha_\nu$  absorption coefficient

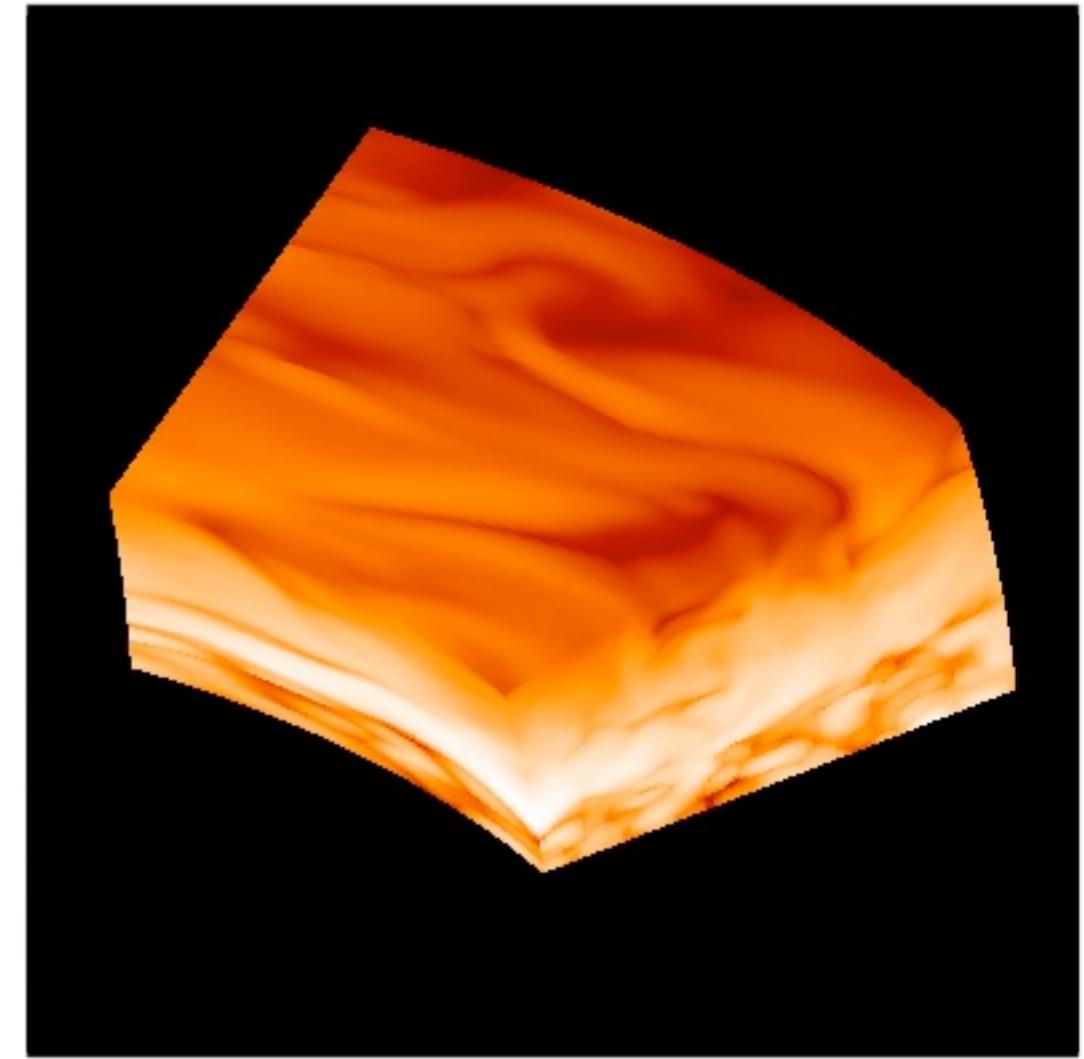
$$I_\nu(\tau_0) = I_\nu(\tau_1)e^{-(\tau_1 - \tau_0)} + \int_{\tau_0}^{\tau_1} S(\tau_\nu)e^{-\tau_\nu} d\tau_\nu$$

# CONTINUUM RADIATIVE TRANSFER

$$j_\nu = \alpha_\nu B_\nu(T_{dust})$$

$$\alpha_\nu = \kappa_\nu \rho_{dust}$$

- popular codes include
  - radmc / radmc-3d (Dullemond)
  - Transphere (Dullemond)
  - DUSTY (Ivezic et al)
  - MC3D (Wolf)
  - HYPERION (Robitaille)



# STATISTICAL EQUILIBRIUM

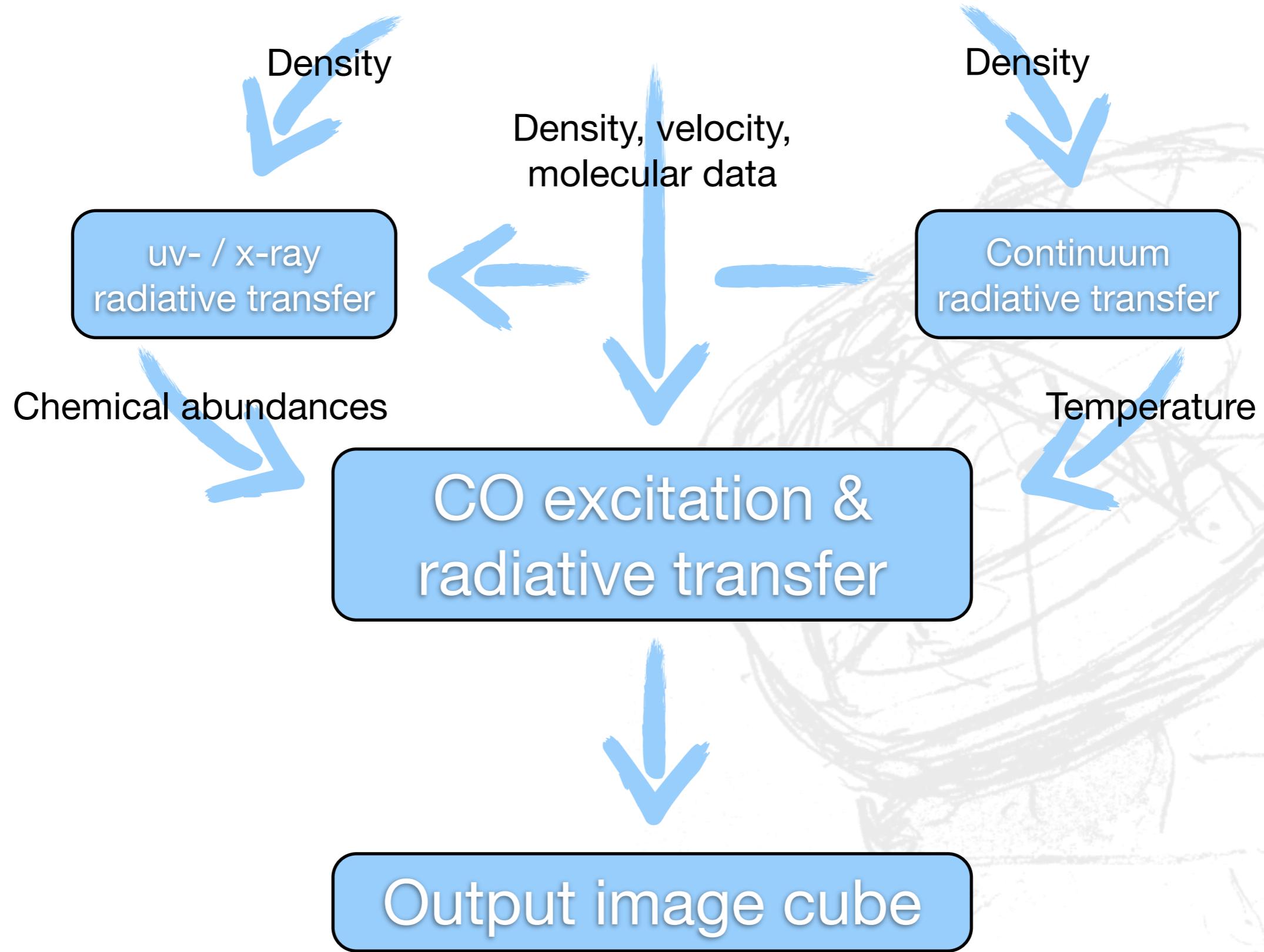
$j_\nu$  and  $\alpha_\nu$  are generally functions of density ( $\varrho$ ), temperature ( $T$ ), opacity ( $\chi$ ), frequency ( $\nu$ ), doppler shifts ( $\phi$ ), Einstein coefficients ( $A_{21}, B_{21}, B_{12}$ ), and quantum level population ( $n$ ).

However,

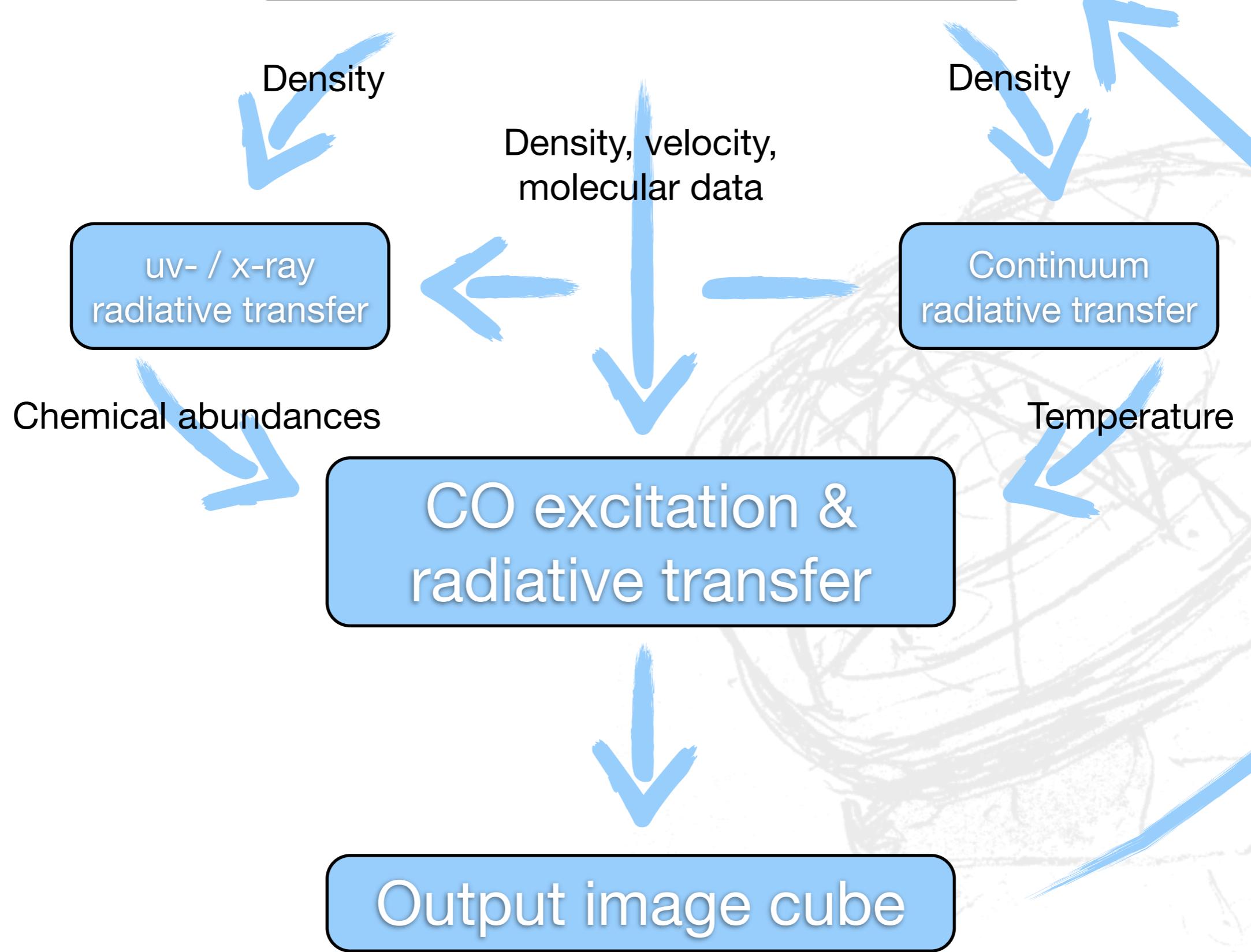
$n$  is a function of the intensity ( $I$ ):

$$n_l \left[ \sum_{k < l} A_{lk} + \sum_{k \neq l} (B_{lk} J_\nu + C_{lk}) \right] = \\ \sum_{k > l} n_k A_{kl} + \sum_{k \neq l} n_k (B_{kl} J_\nu + C_{kl}).$$

# Input model



# Input model



# WHY IS RADIATIVE TRANSFER HARD?

Simon Bruderer says:

Given

n cells (10000)

r lines (100)

s frequencies (100)

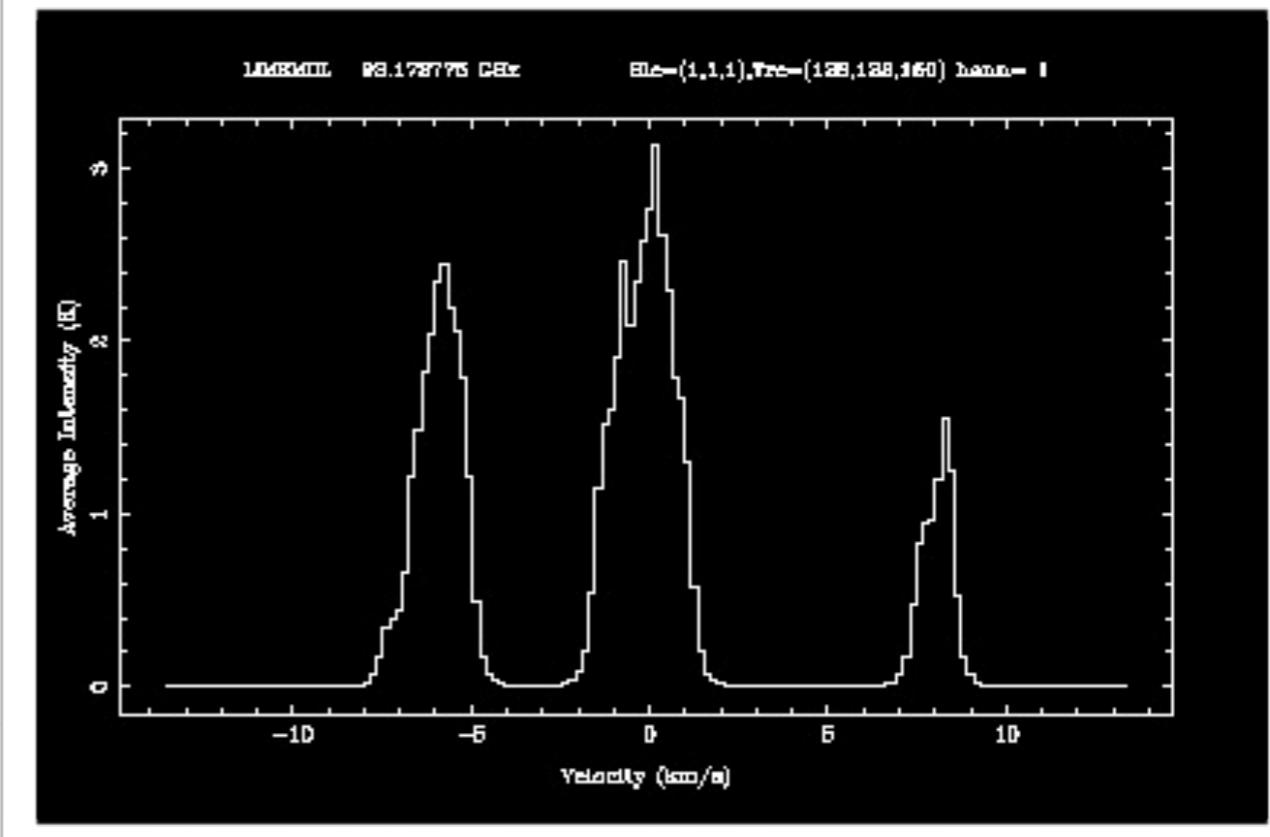
$n^2 \times r \times s = 1e12$  radiative connections

On one 2 GHz cpu, `exp()` takes of order ~ 30ish cycles  
=> 5e7 `exp()`/second

$1e12 \text{ exp()}/\text{iteration} / 5e7 \text{ exp()}/\text{second} = 20000 \text{ seconds}$   
(or 6 hours) / iteration

# MOLECULAR EXCITATION AND LINE RADIATIVE TRANSFER

- Exact methods
  - LI
  - ALI
  - MC
  - AMC
  - ...
- Approximations
  - LTE
  - Escape probability method
  - Large Velocity Gradient
  - ...



# MOLECULAR EXCITATION AND LINE RADIATIVE TRANSFER

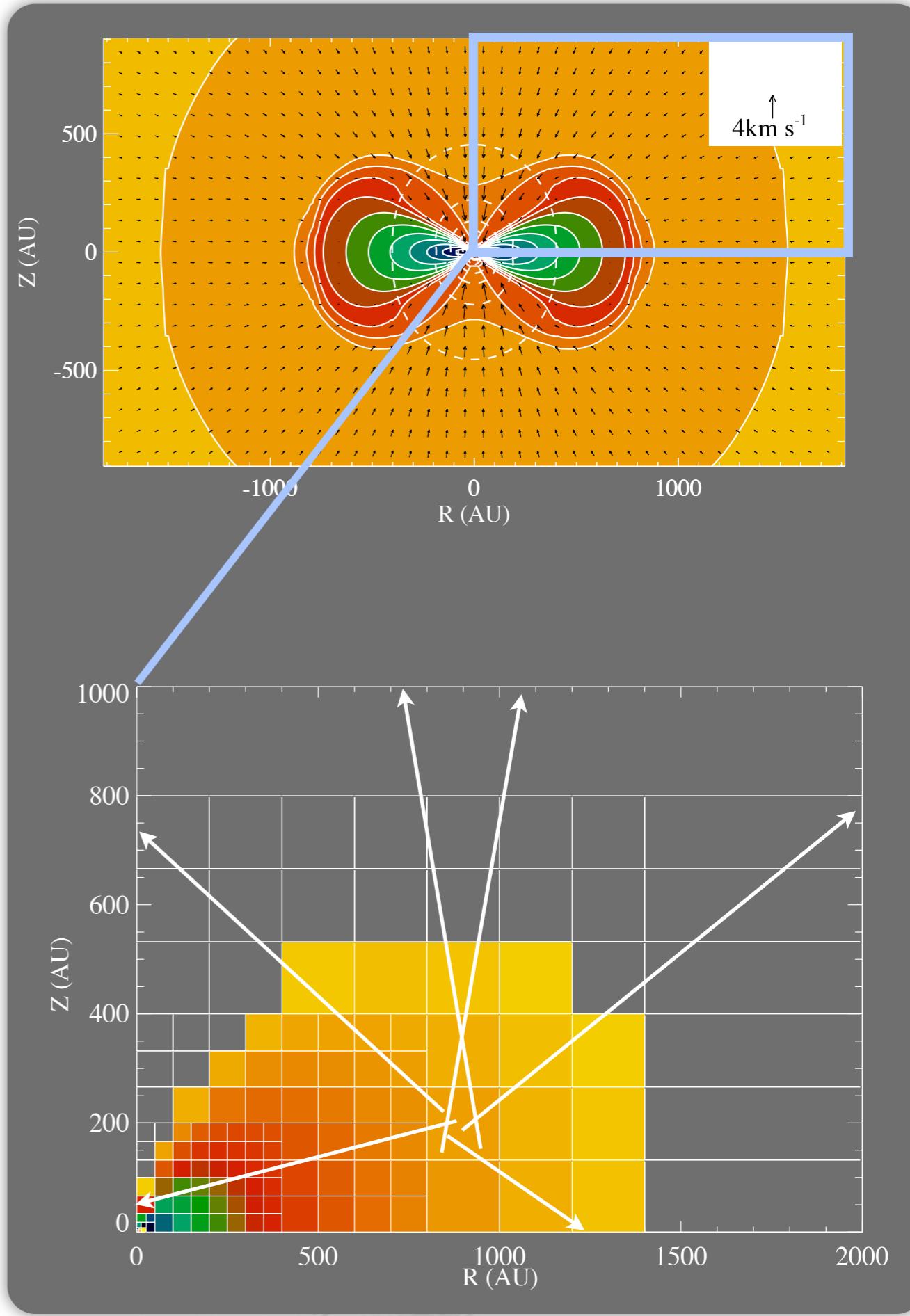
∀ cell:

trace n photon in  
random directions

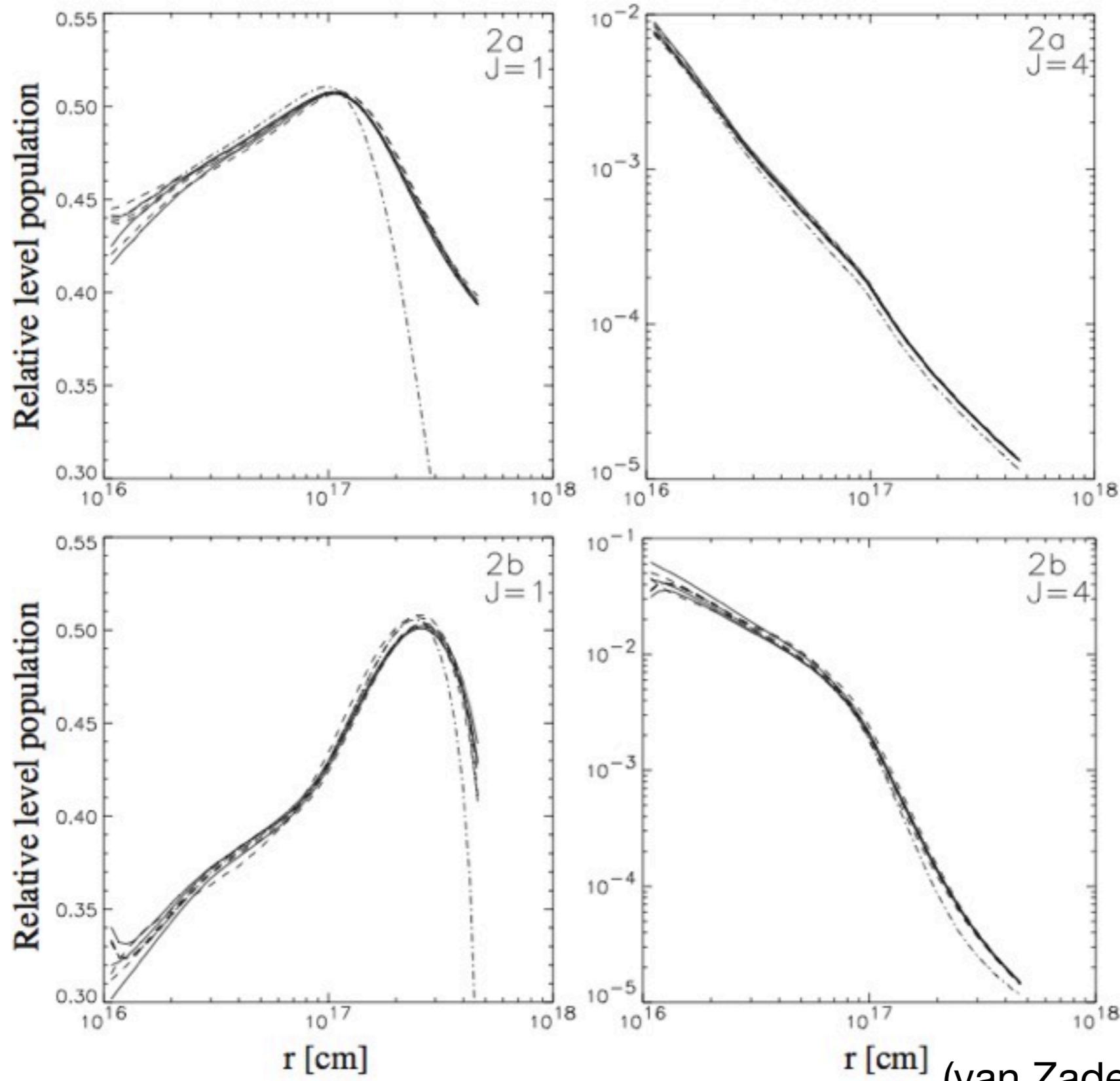
Calculate mean  
radiation field seen  
by cell

Construct rate matrix

Solve for populations



# BENCHMARK

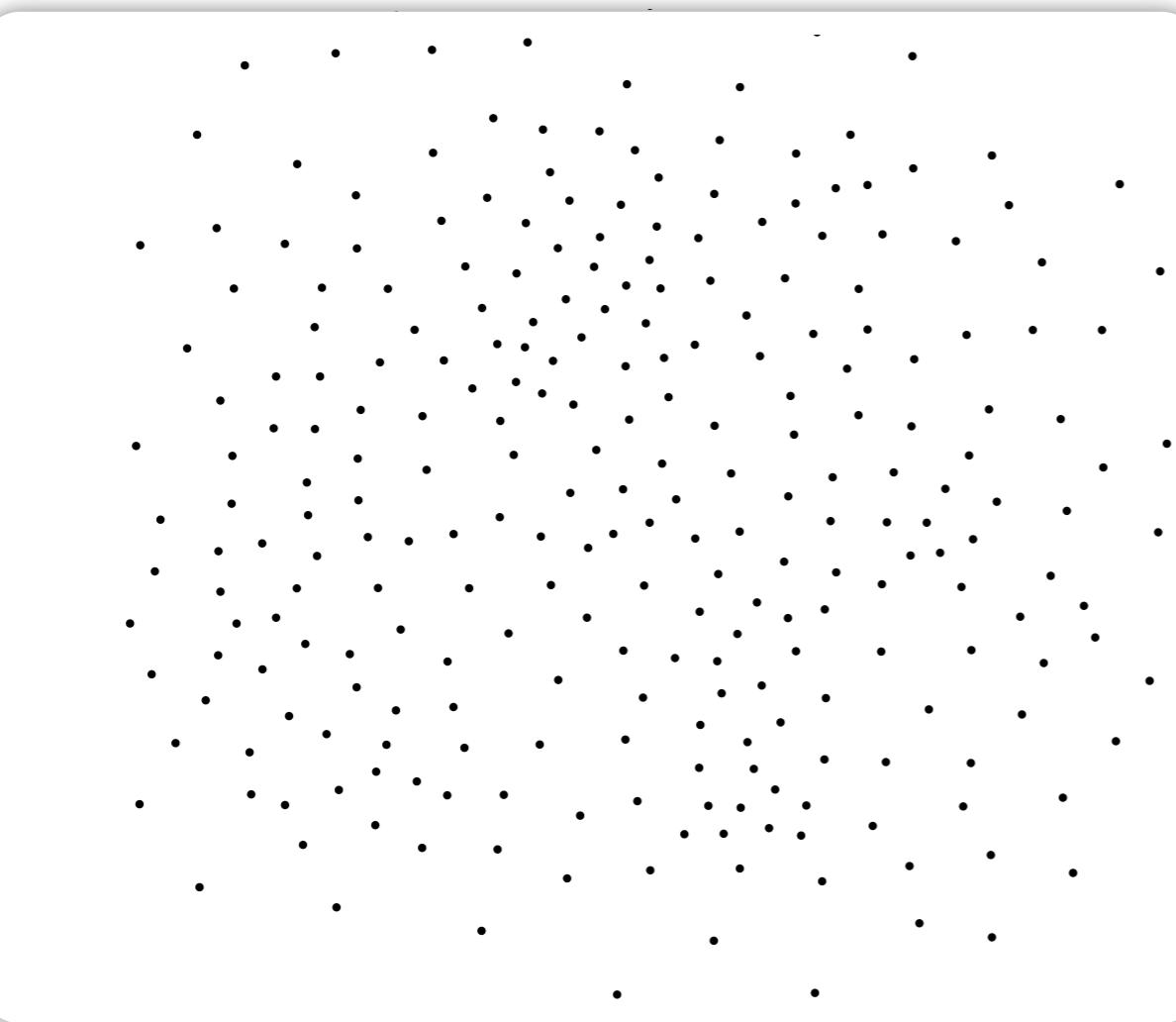


(van Zadelhoff et al., 2002)

# PITFALLS

- Describing the model on a computational grid is (always!) difficult
- Convergence can be an issue
- The velocity field problem
- Parameters for imaging / ray-tracing need to be chosen carefully

# LINE MODELING ENGINE (LIME)



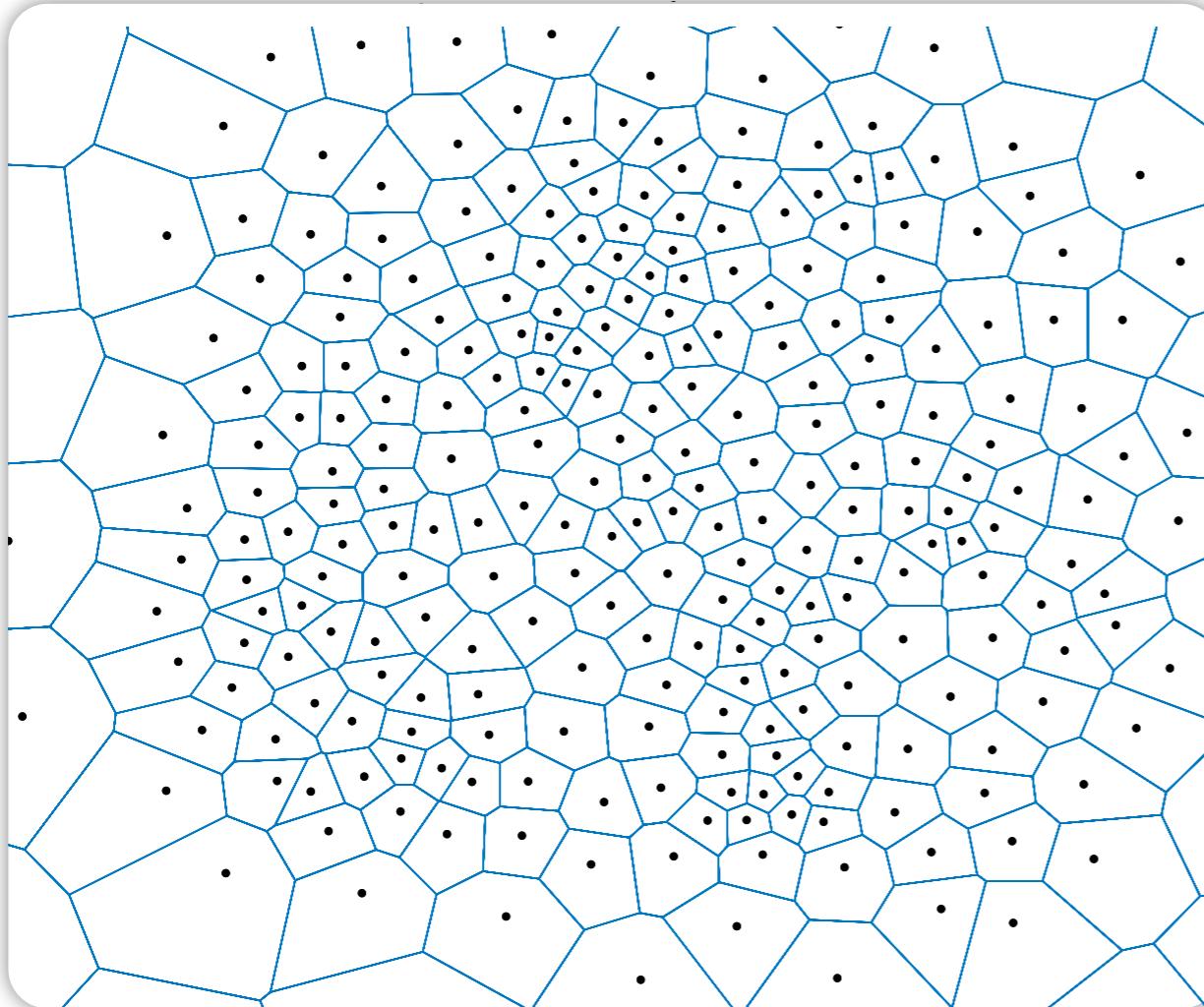
- 3D line radiative transfer
- Random Delaunay grids for fast photon transfer
- Model properties are constant over a Voronoi volume (=> automatic mass conservation)



(Brinch and Hogerheijde, 2010)



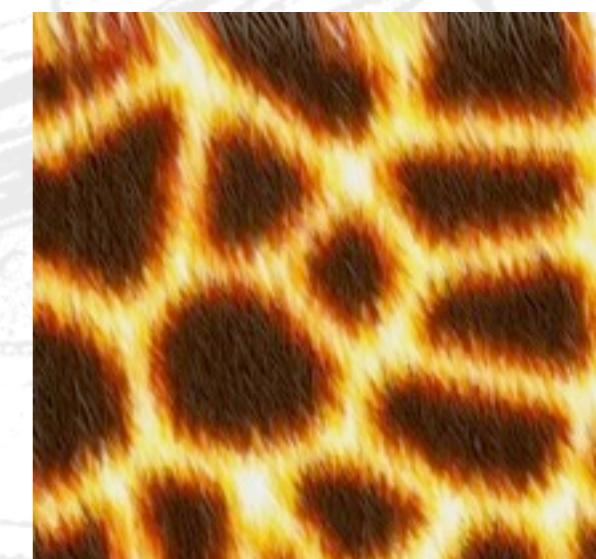
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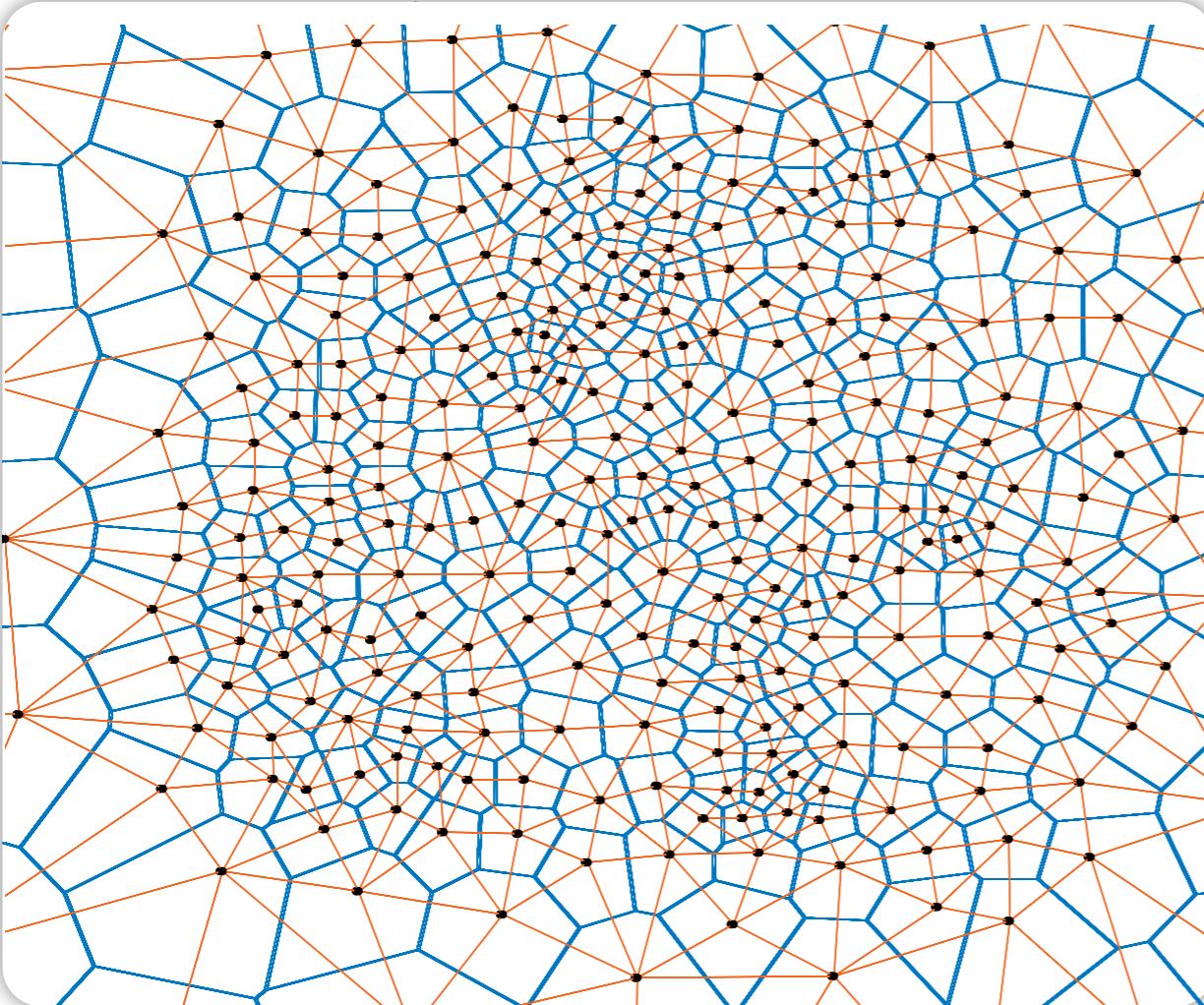
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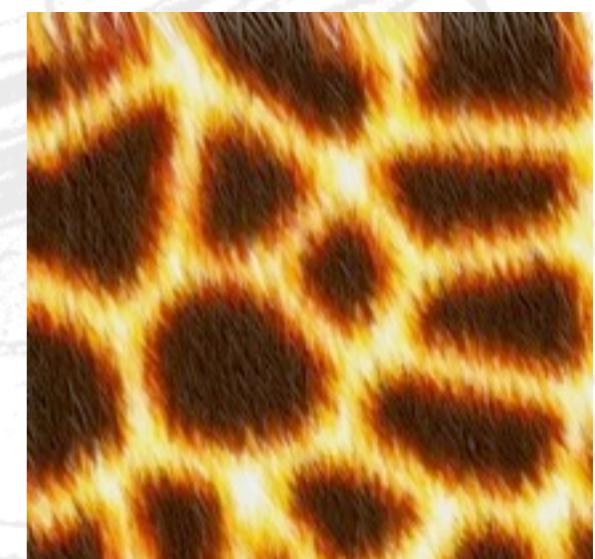
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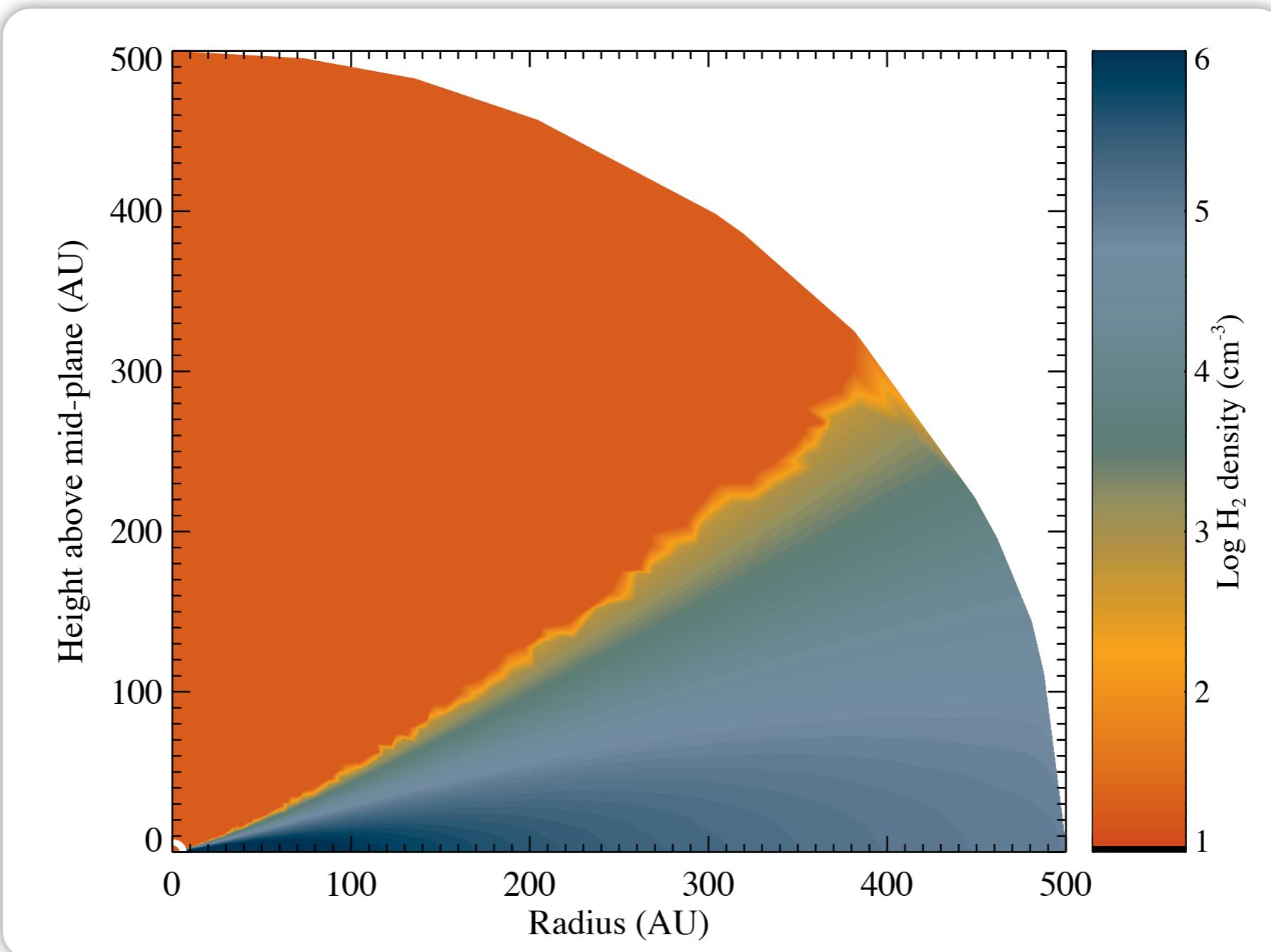
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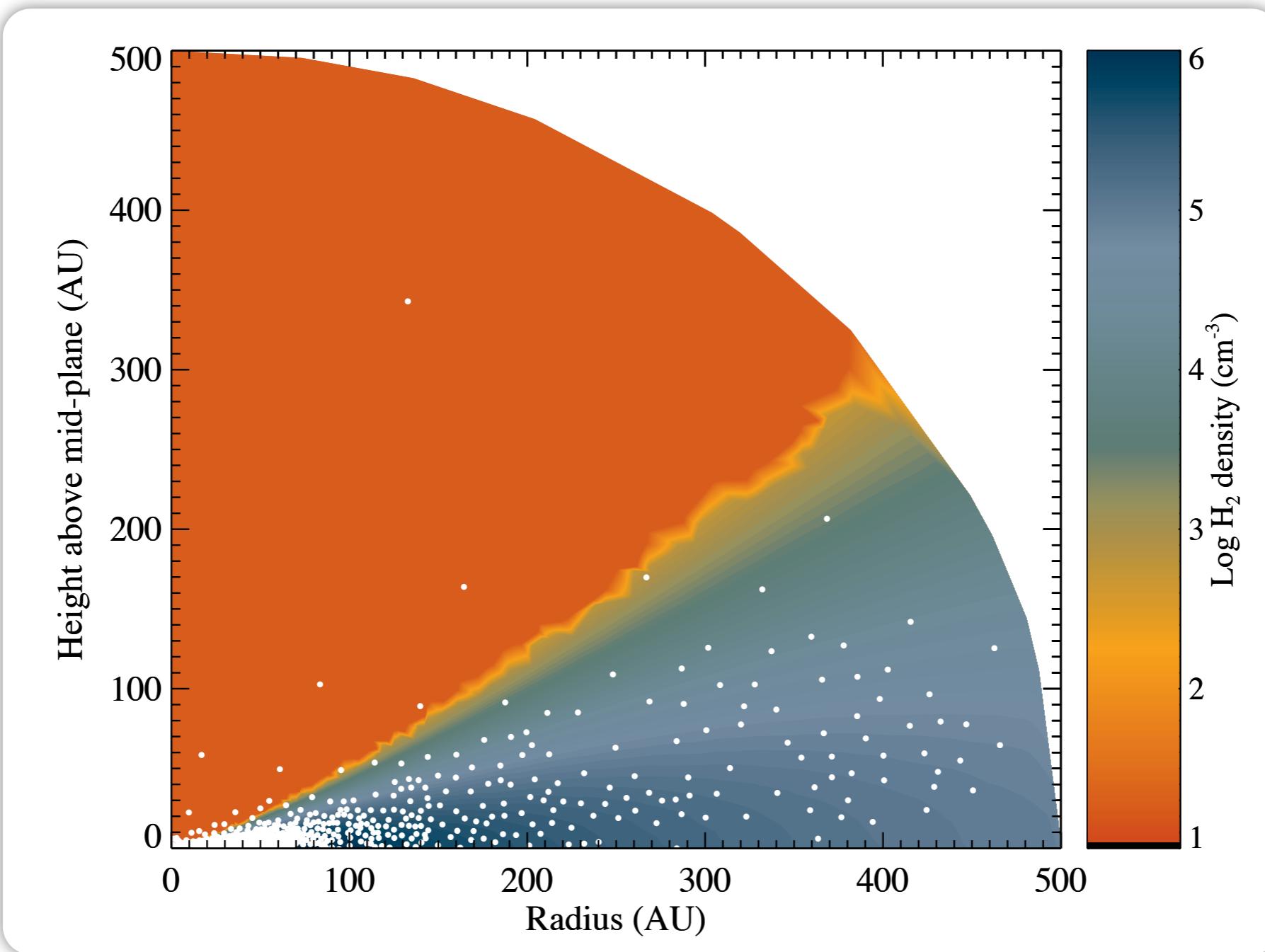
(Brinch and Hogerheijde, 2010)



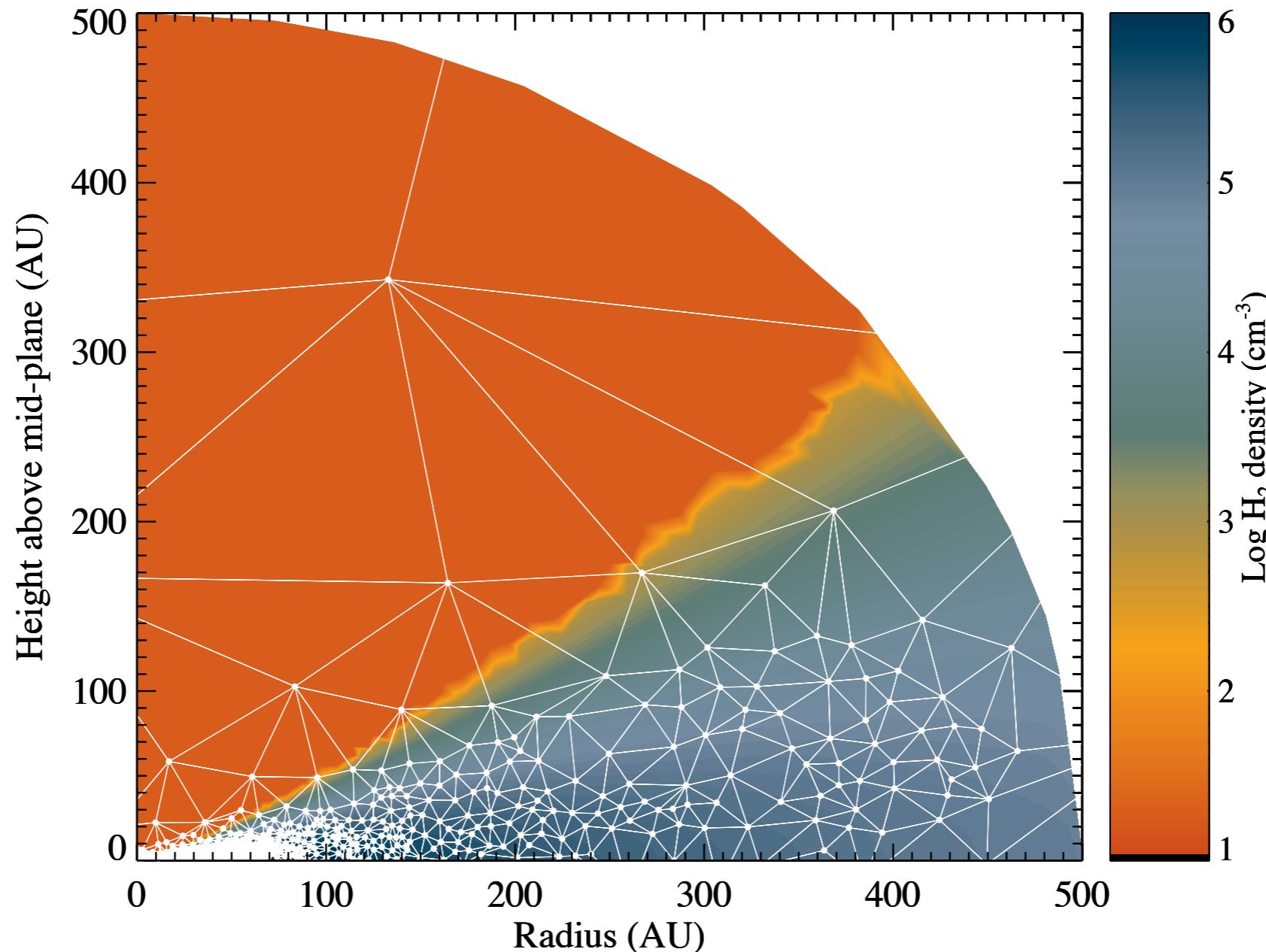
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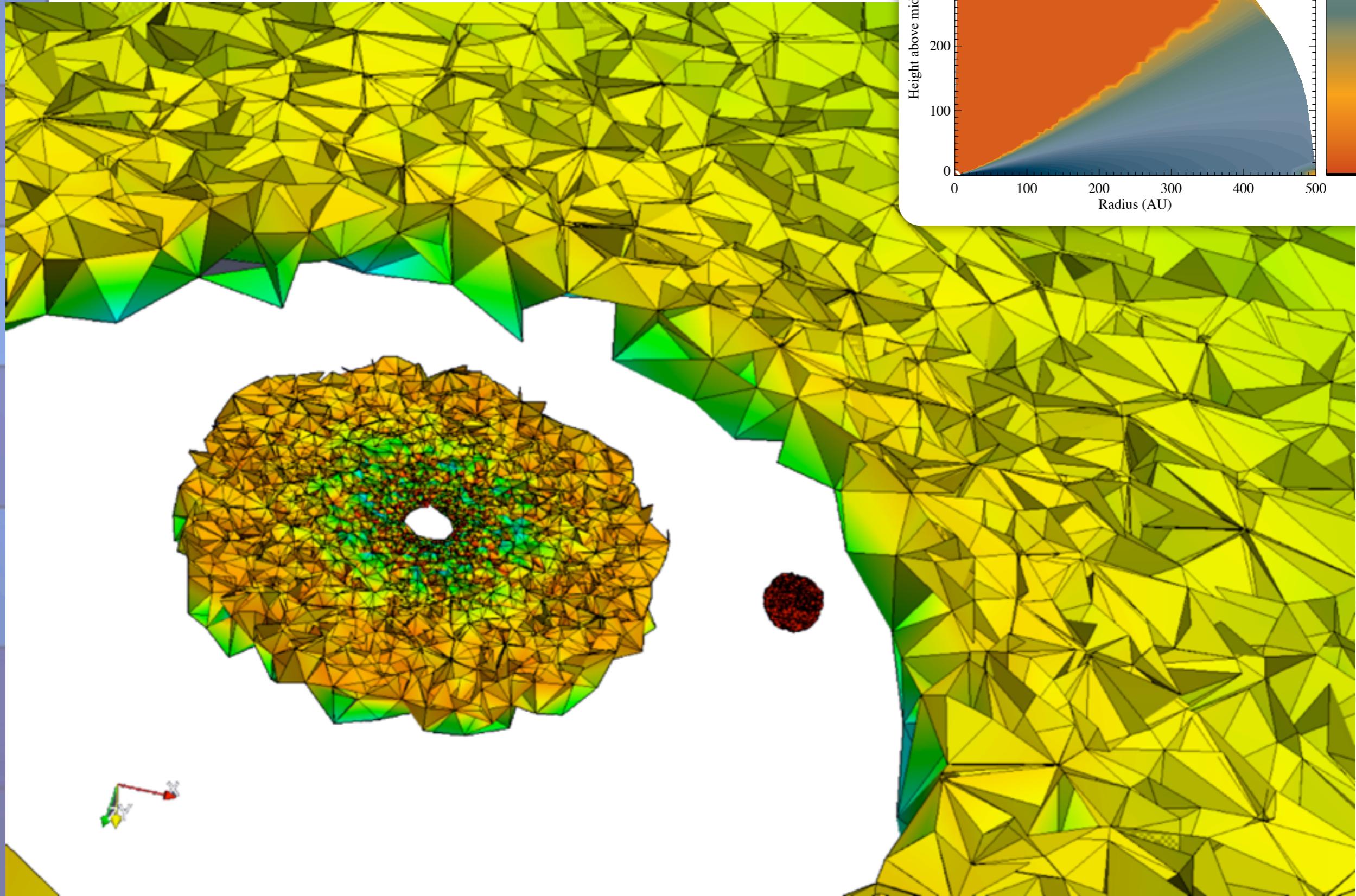
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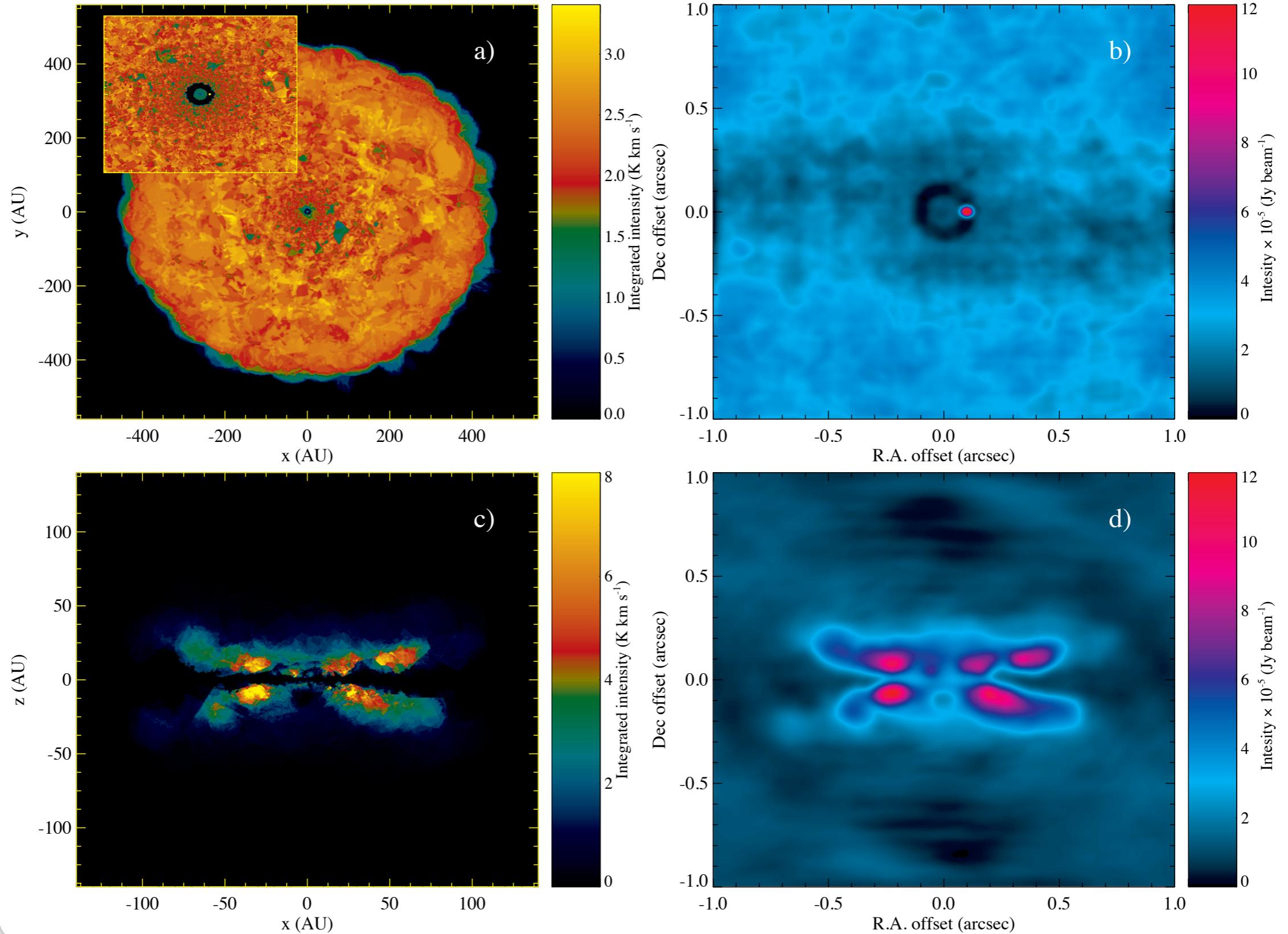
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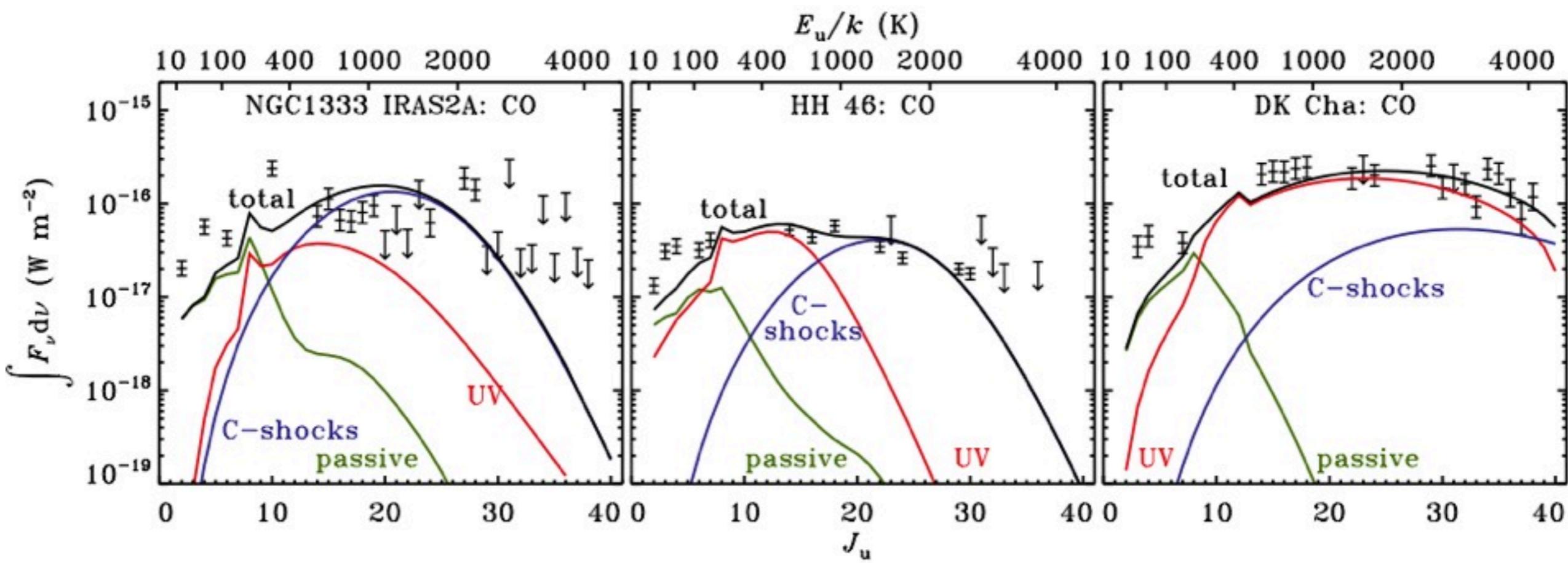
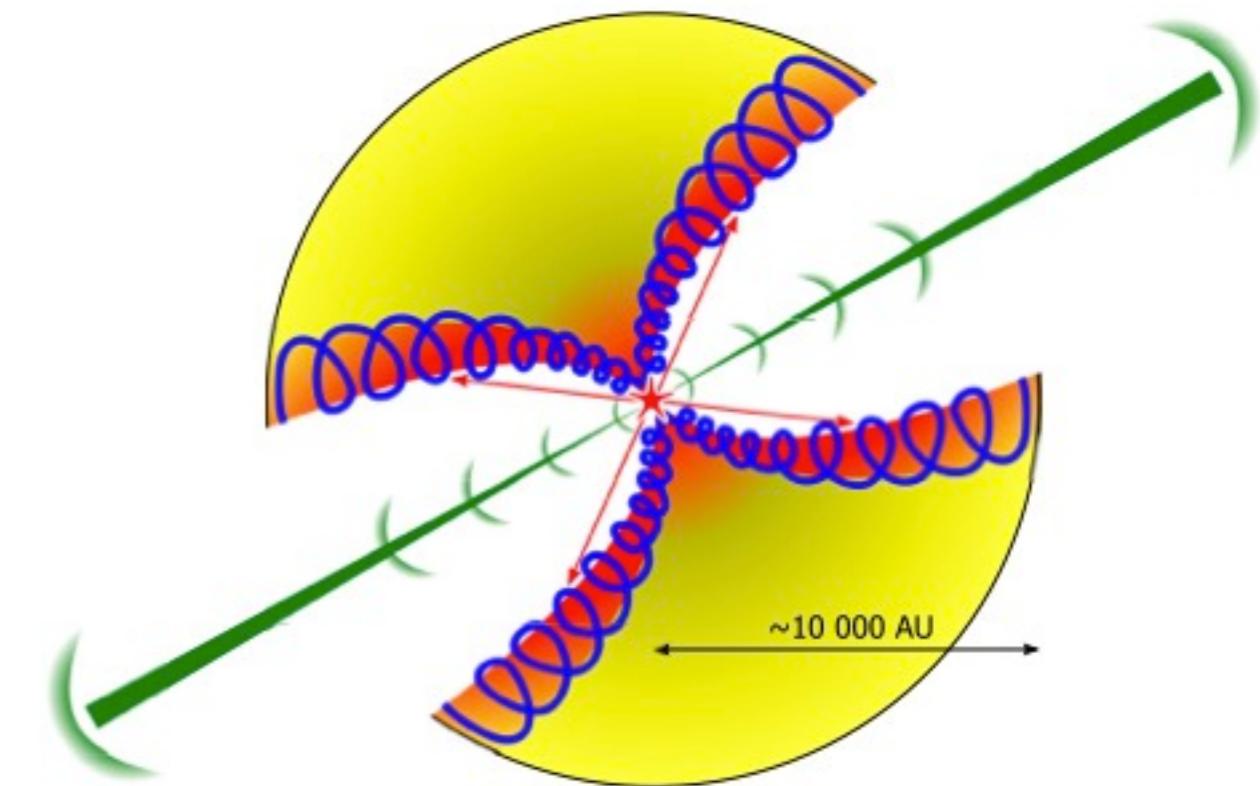
# 3D PROTOPLANETARY DISK WITH A PROTOPLANET



# 3D PROTOPLANETARY DISK WITH A PROTOPLANET



# HOT CO IN YSOs



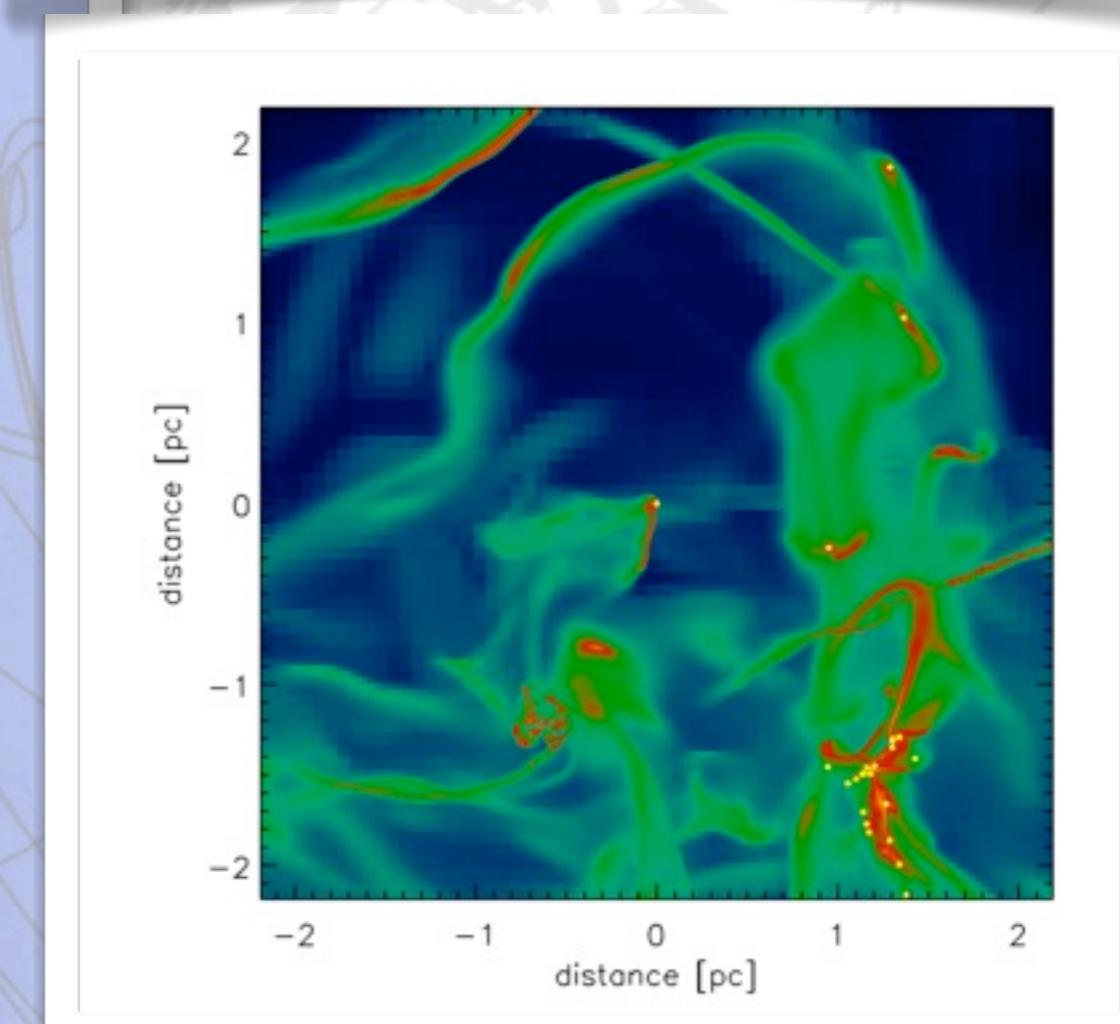
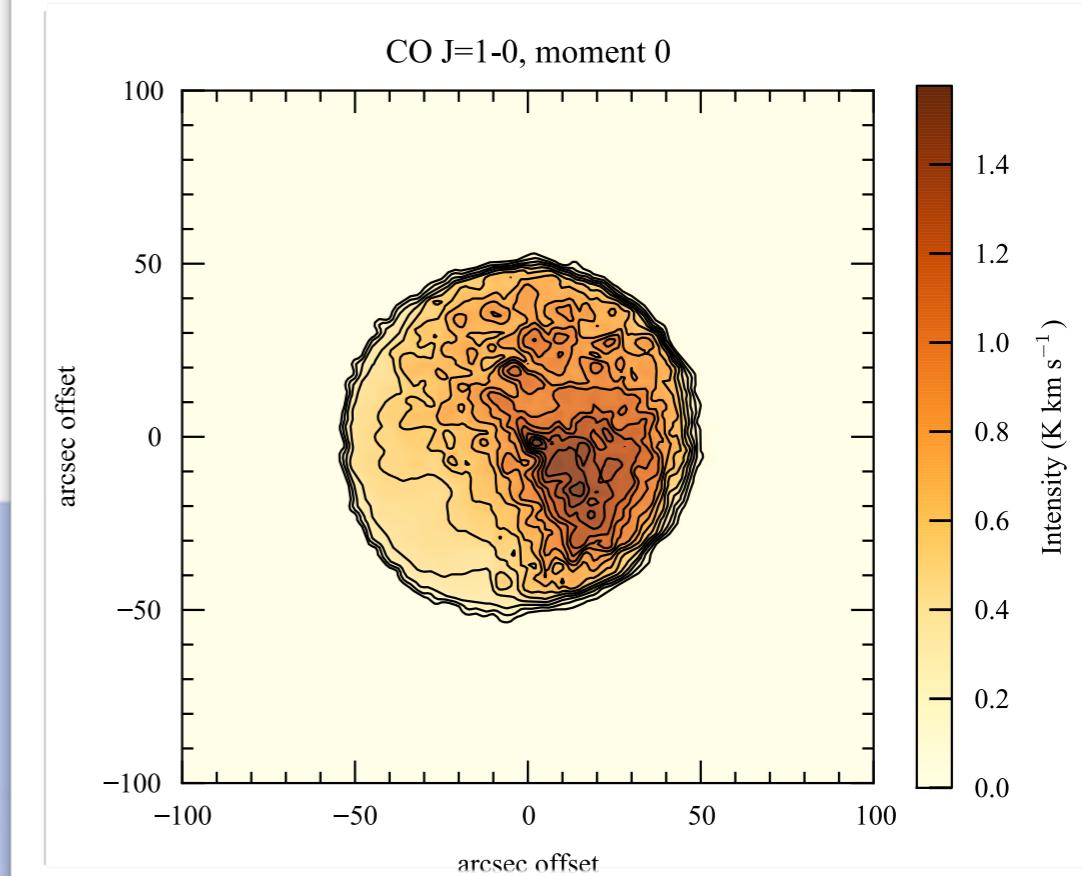
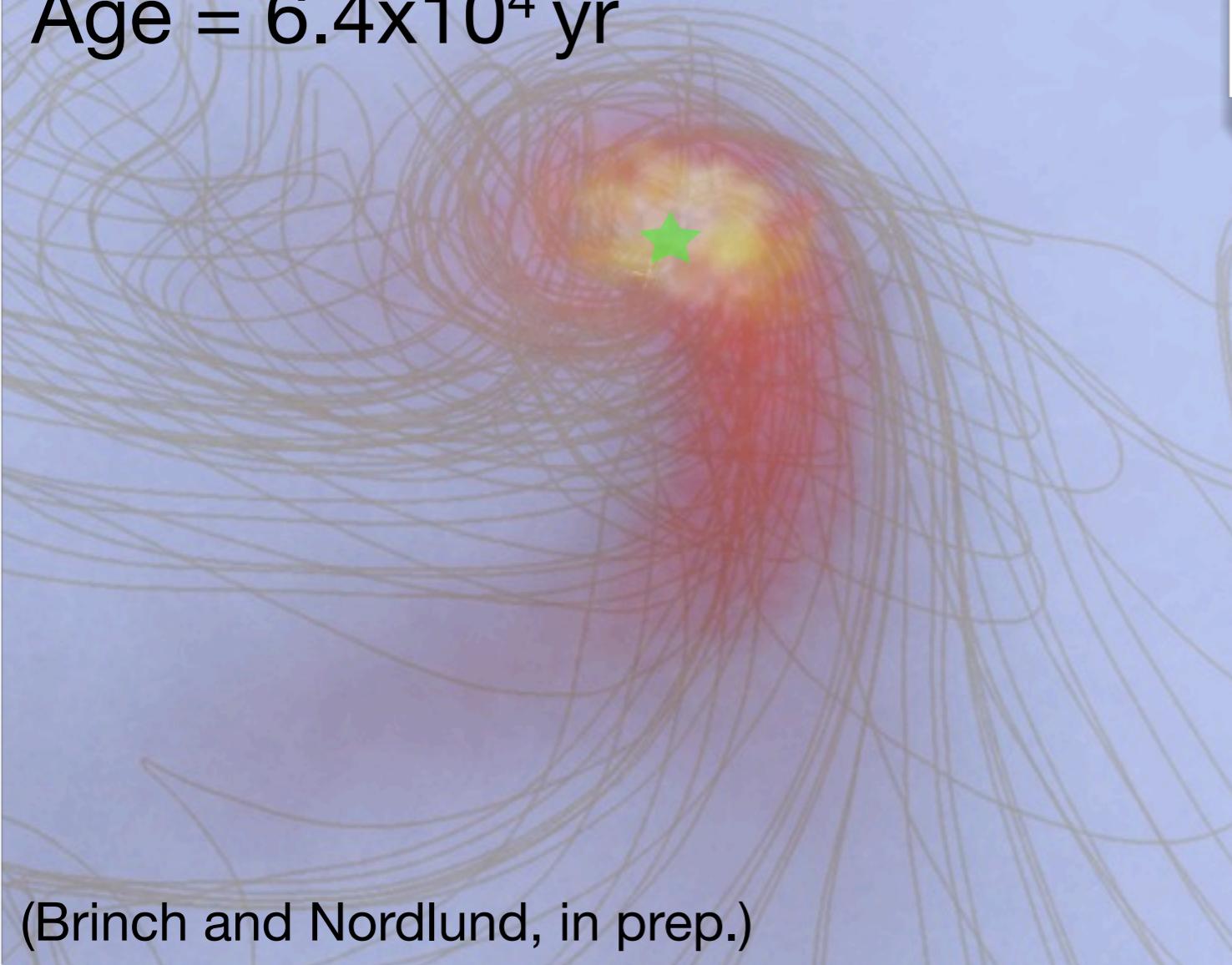
(Visser et al., 2012)

# NUMERICAL SIMULATIONS AND RADIATIVE TRANSFER

Star #283

Mass =  $0.8 M_{\odot}$

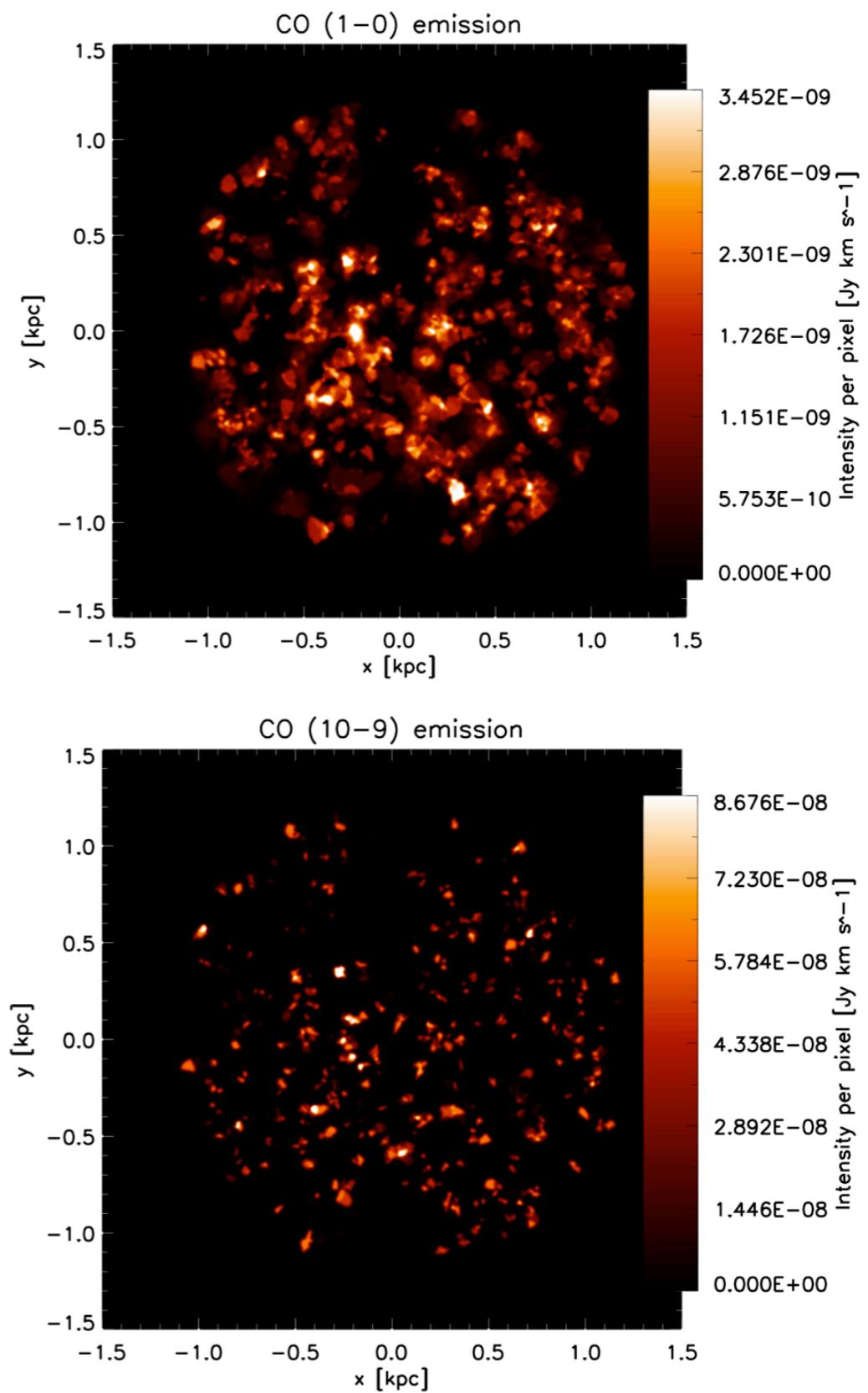
Age =  $6.4 \times 10^4$  yr



# RADIATIVE TRANSFER CALCULATIONS ON MODELS OF GALAXIES

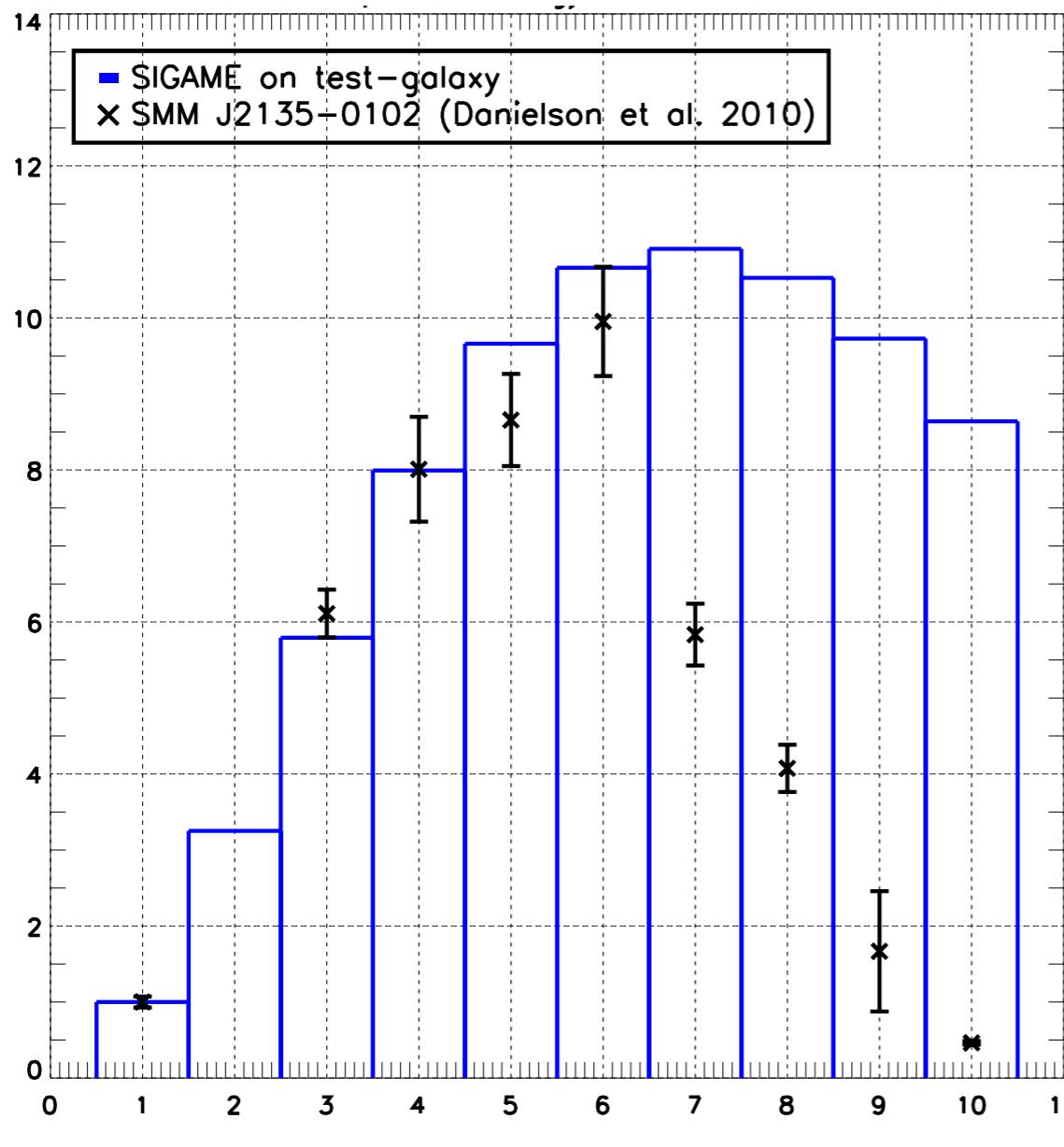


See poster by Karen Pardos Olsen

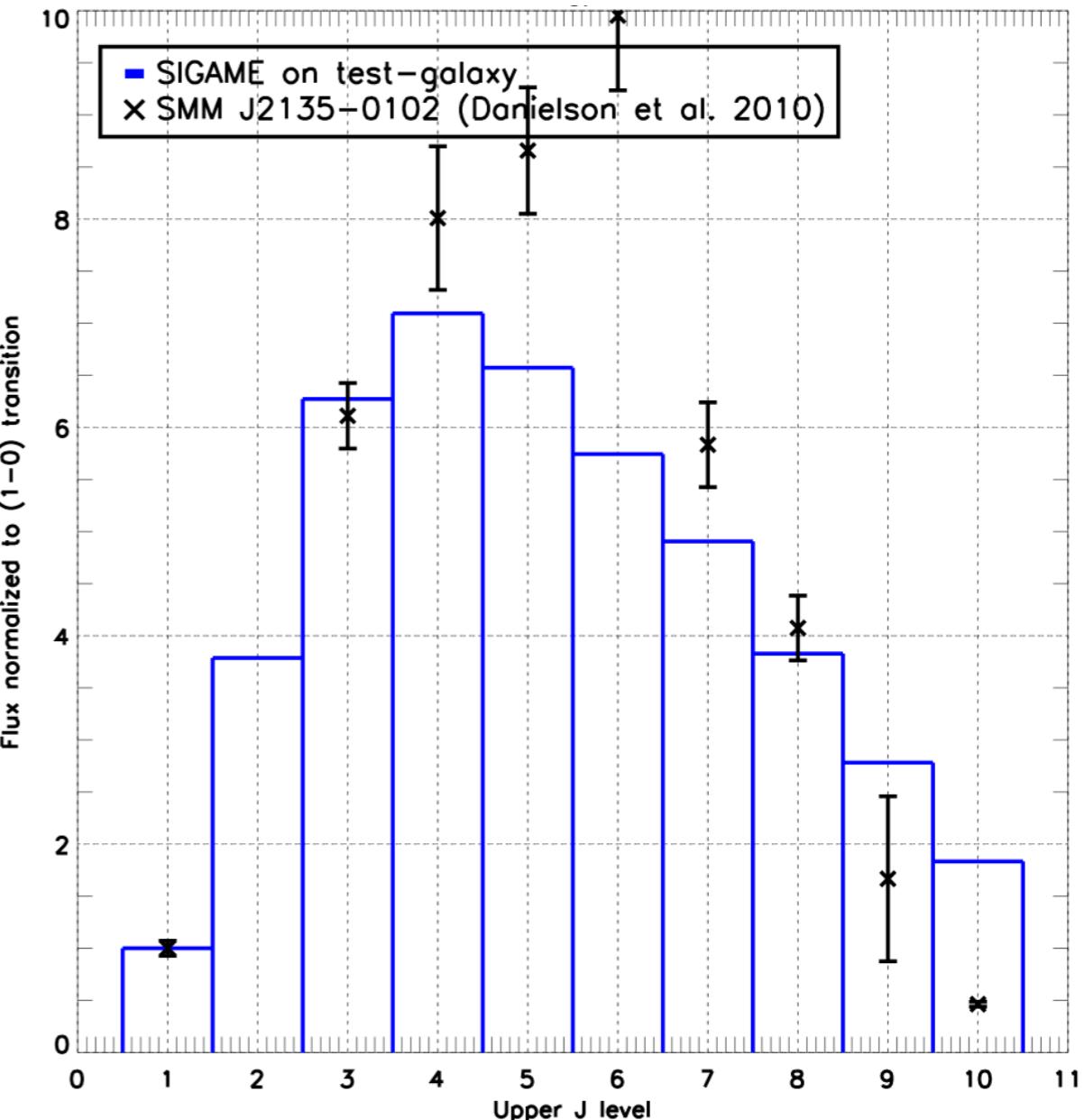


# RADIATIVE TRANSFER CALCULATIONS ON MODELS OF GALAXIES

T=30K



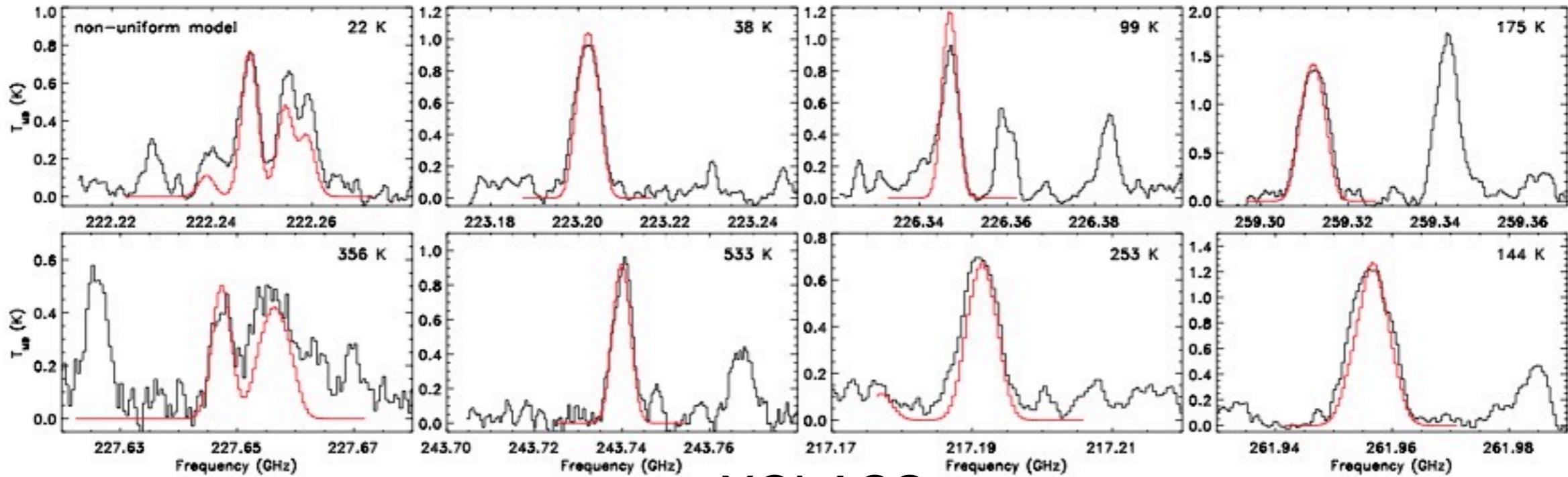
T=20K



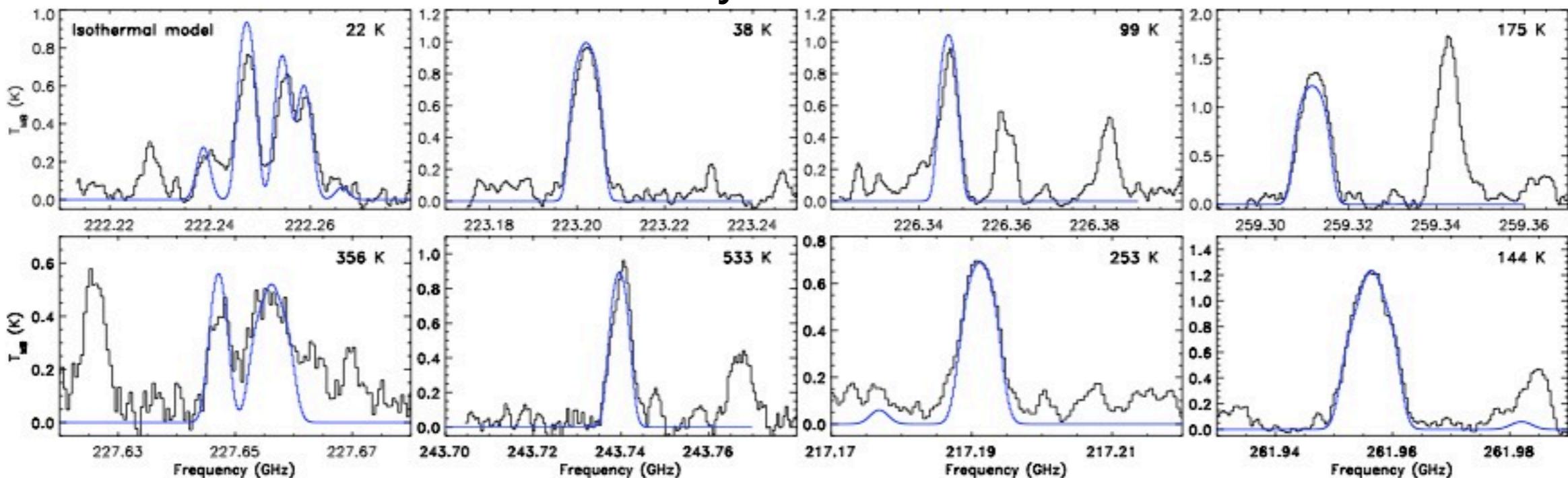
See poster by Karen Pardos Olsen

# HIGH-RESOLUTION COMPLEX ORGANICS

LIME



myXCLASS



(Bisschop et al., submitted)

# CONCLUDING REMARKS

- ★ Pick a code that is best suited to solve your particular problem.
- ★ Radiative transfer modeling is (can be) very difficult, but the solutions are usually robust.
- ★ High dimensional radiative transfer require high dimensional input models (where are the theorists?)