High-resolution 3D models of photodissociation regions

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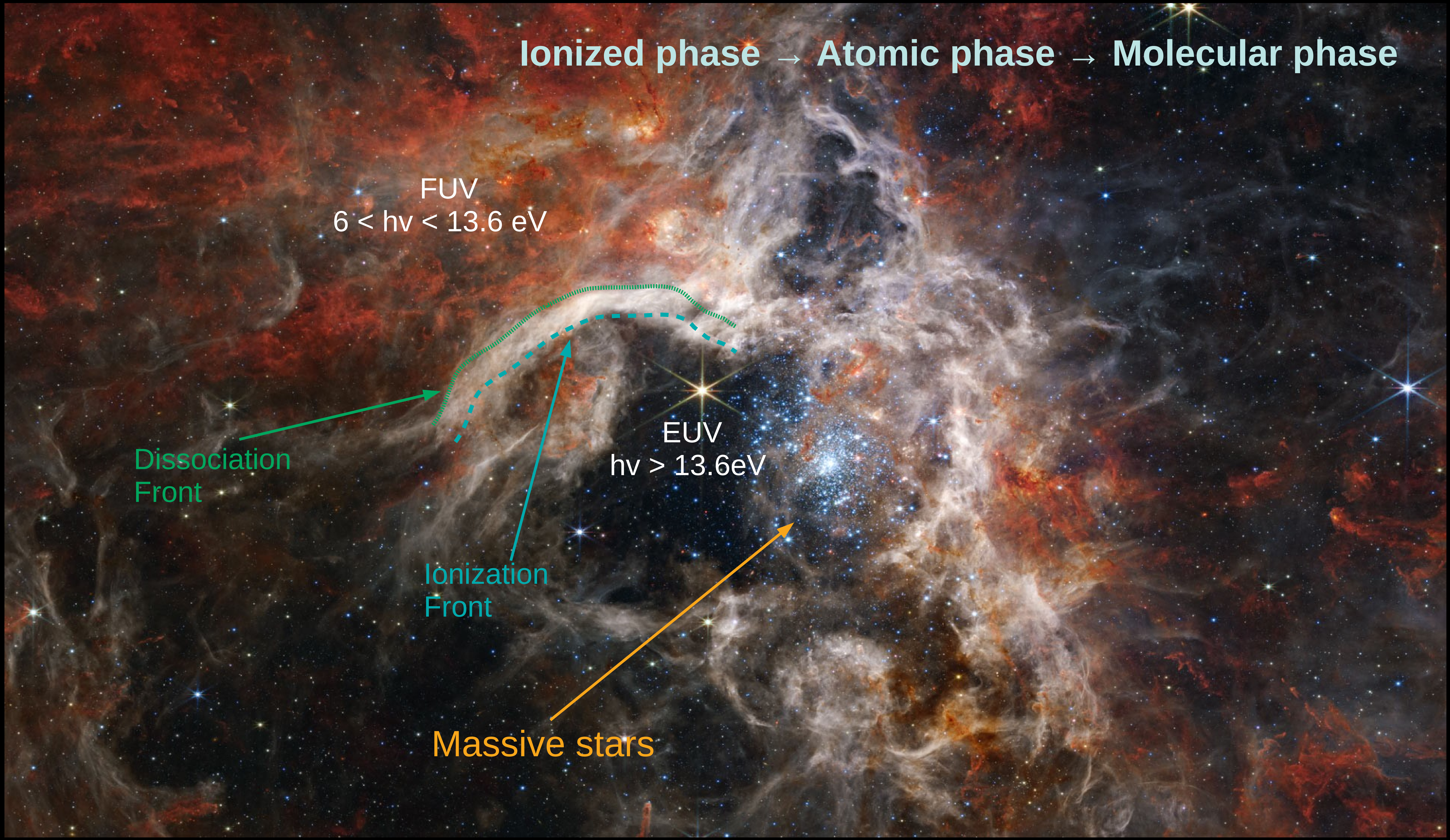
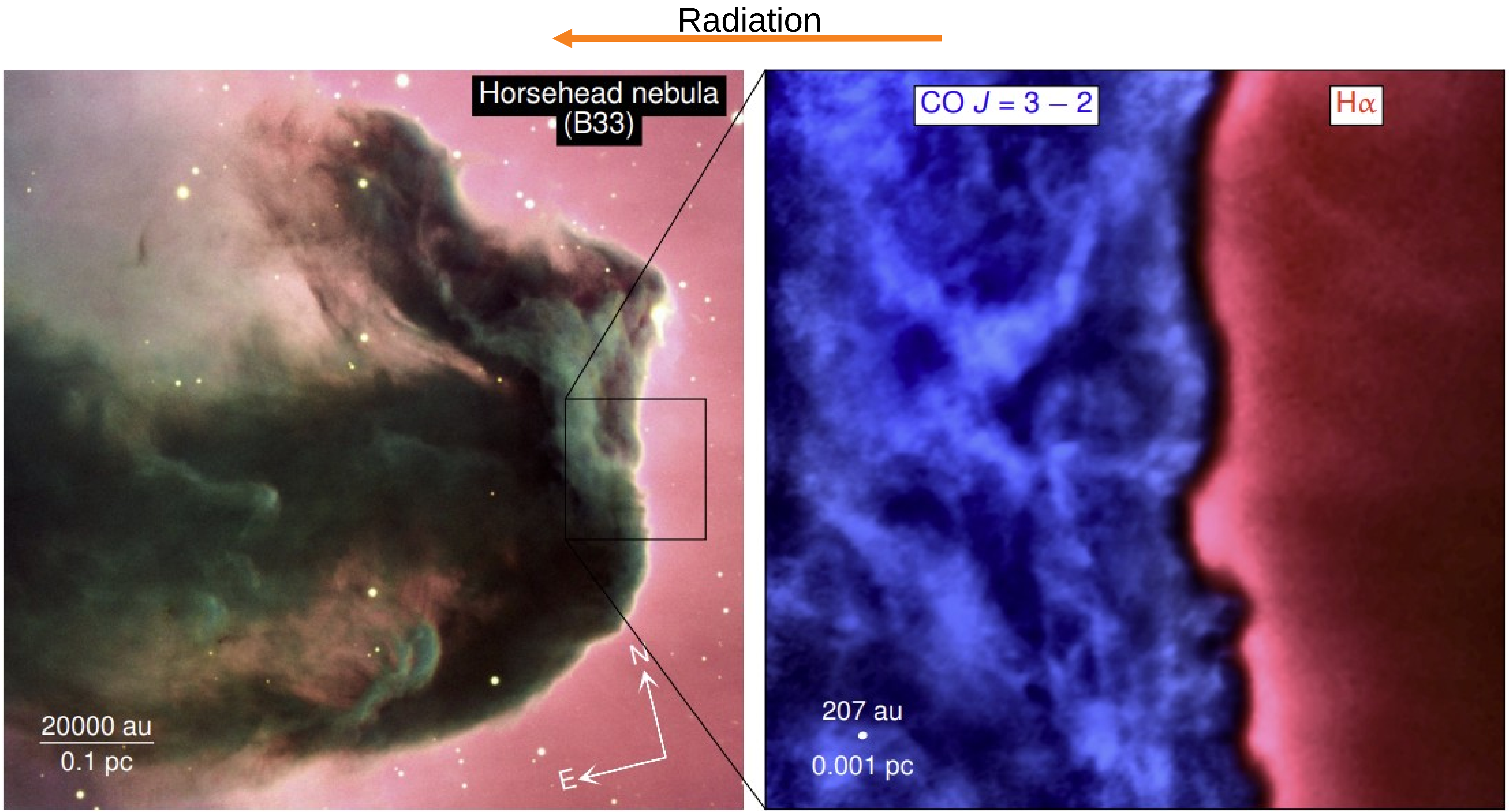
Tarantula Nebula



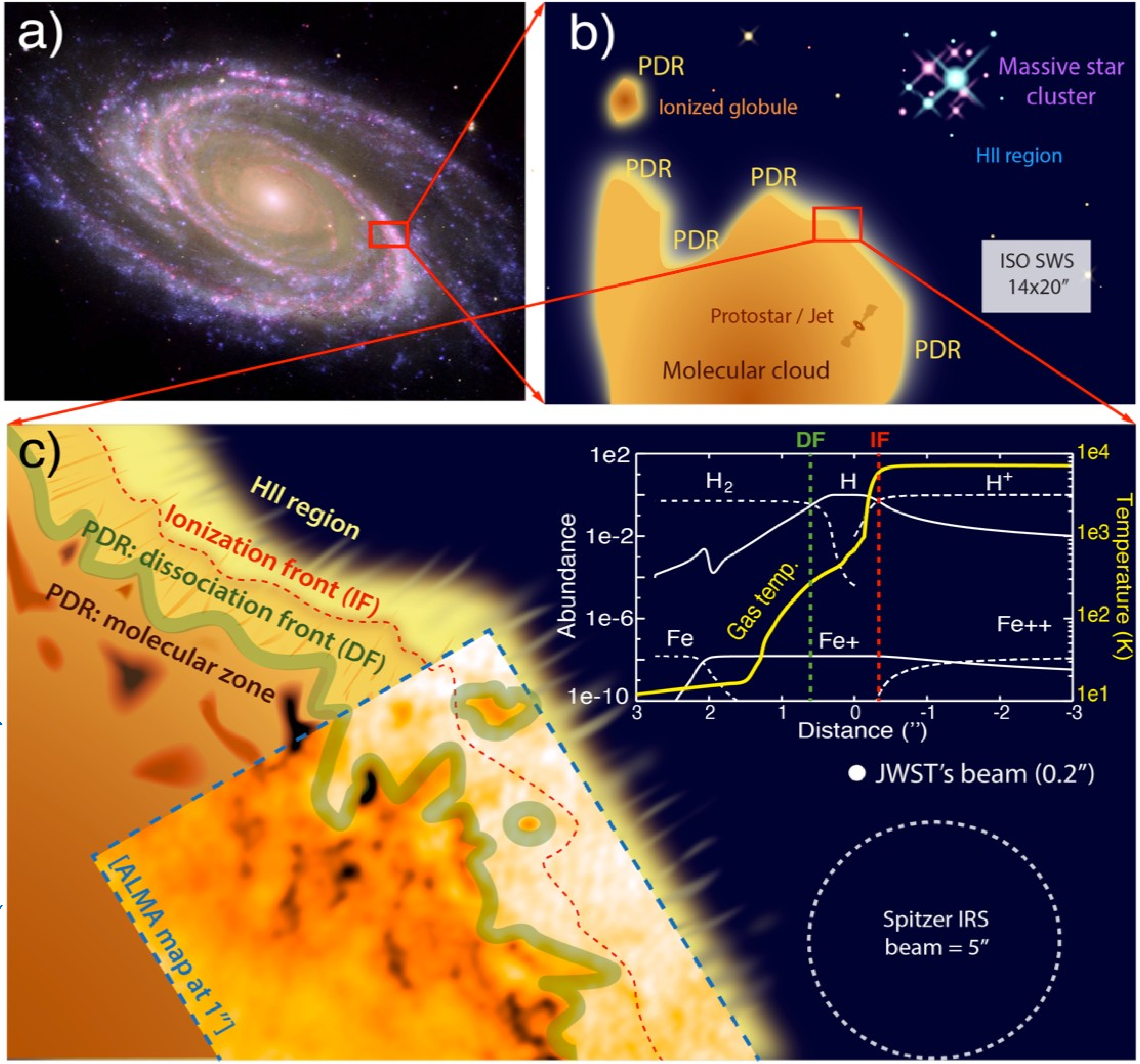
Photodissociation Regions (PDRs)



Hernandez-Vera+ (2023)

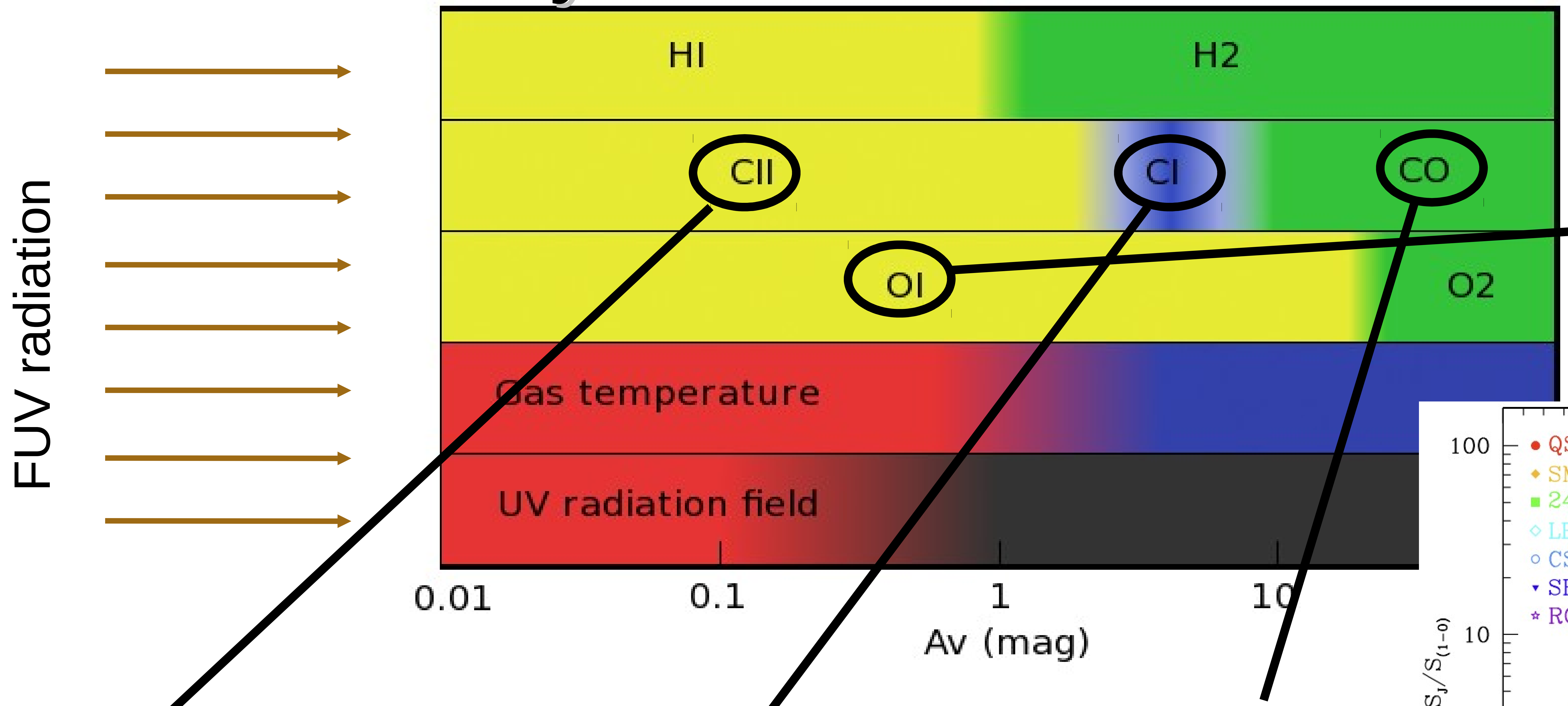
Photodissociation Regions

A large fraction of the ISM is associated with PDRs



PDRs4all (Berne+ 2022)

The carbon cycle and the HI-to-H2 transition

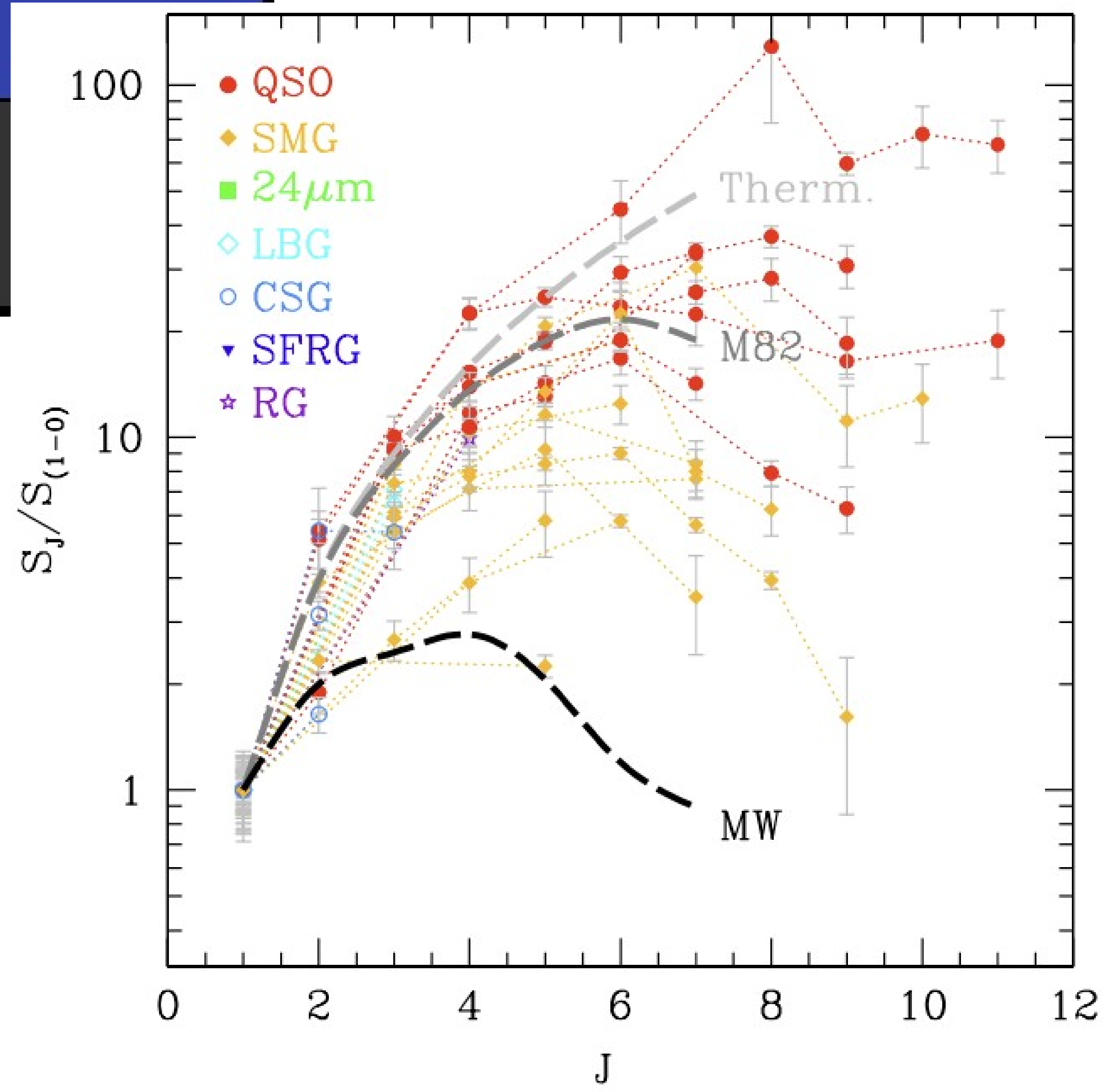


[OI] 63 μm
[OI] 146 μm

[CII] 158 μm

[CI](1-0) 609 μm
[CI](2-1) 370 μm

CO J=1-0
CO J=2-1
CO J=3-2 …



Carilli & Walter (2013)

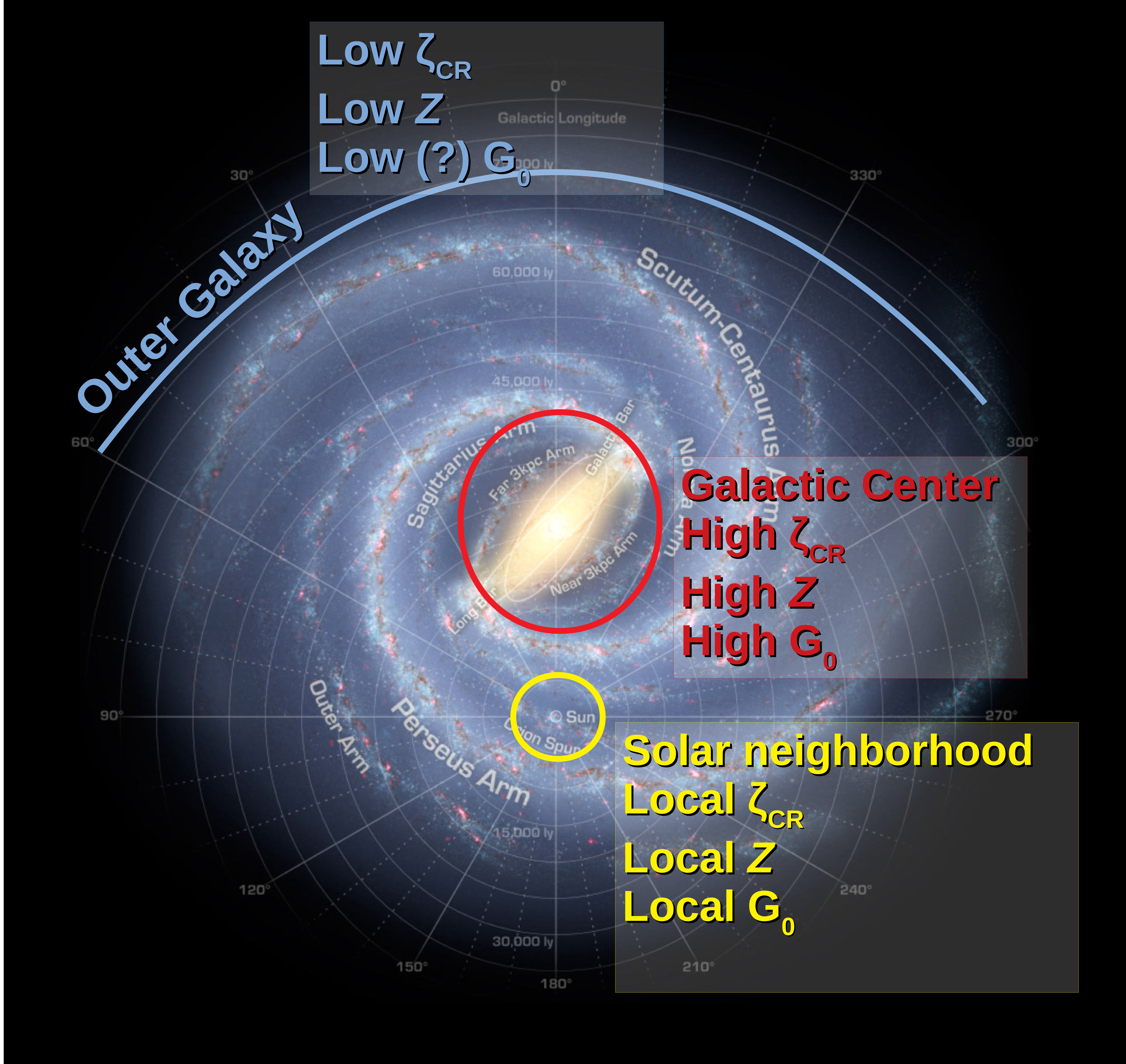
The higher the transition, the denser the ISM it traces.

ISM environmental parameters

"*Extreme*" defined in contrast to the more "*typical*" ISM environments

- ✓Radiation Field
- ✓Gas temperature
- ✓Density
- ✓Cosmic-ray flux
- ✓X-ray flux
- ✓Metallicity
- ✓Shocks

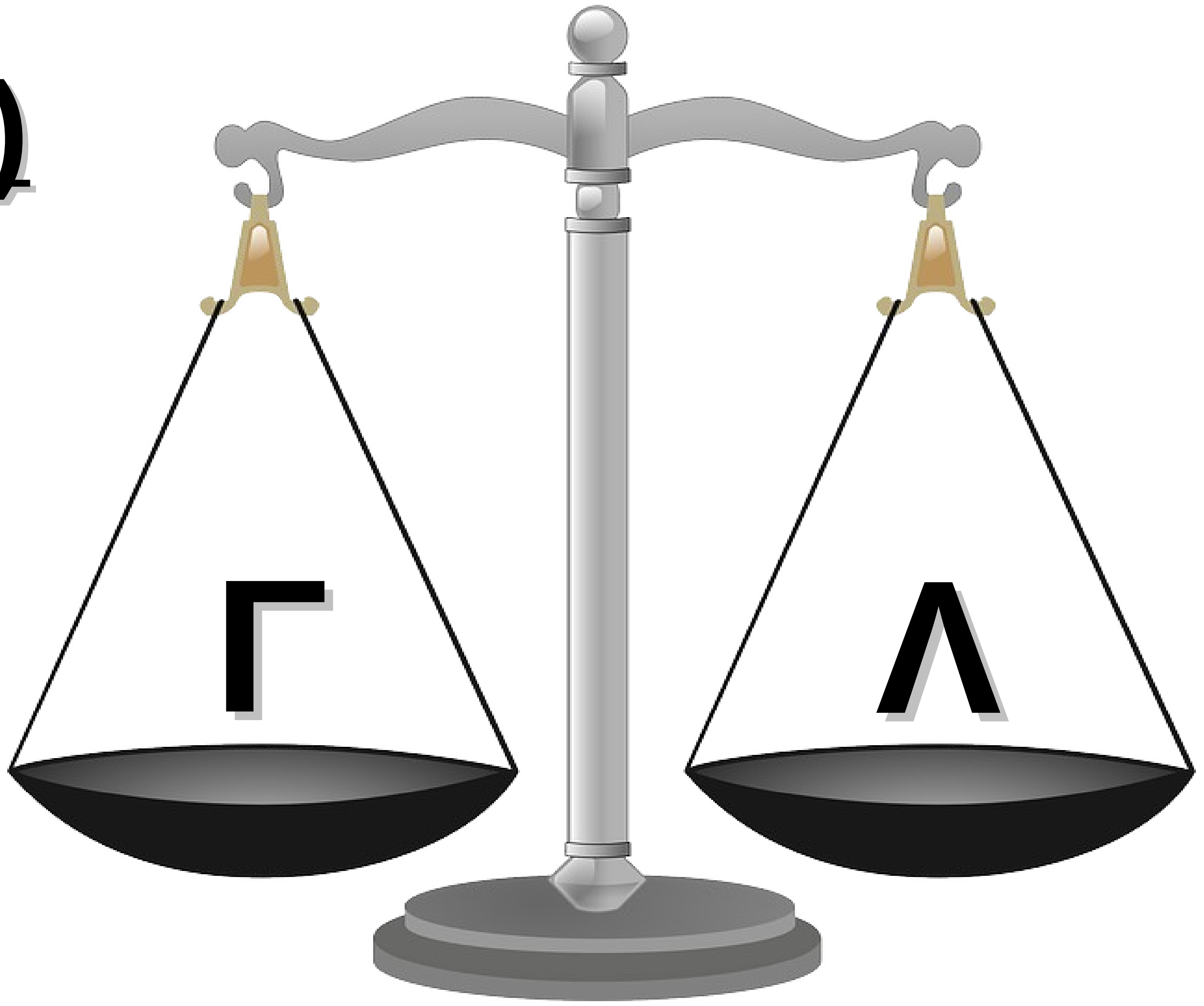
...etc



What controls the thermal balance in PDRs?

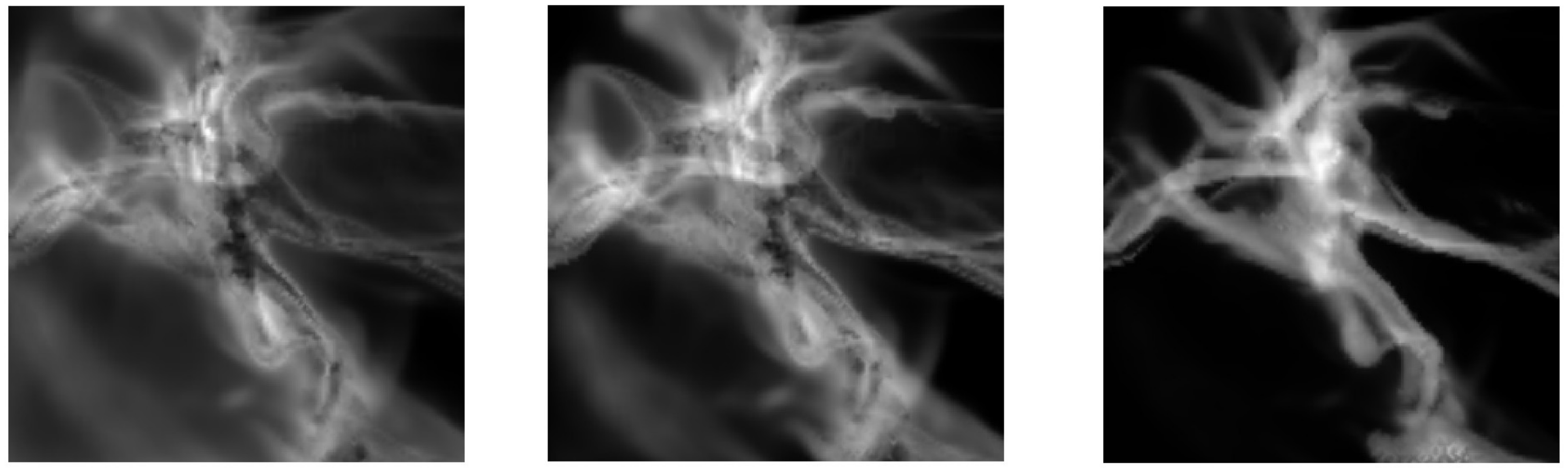
Heating functions (Γ)

- Photoelectric heating
- H_2 formation heating
- Cosmic-ray heating
- X-ray heating
- Shock heating
- Exothermic reactions (“chemical”) heating

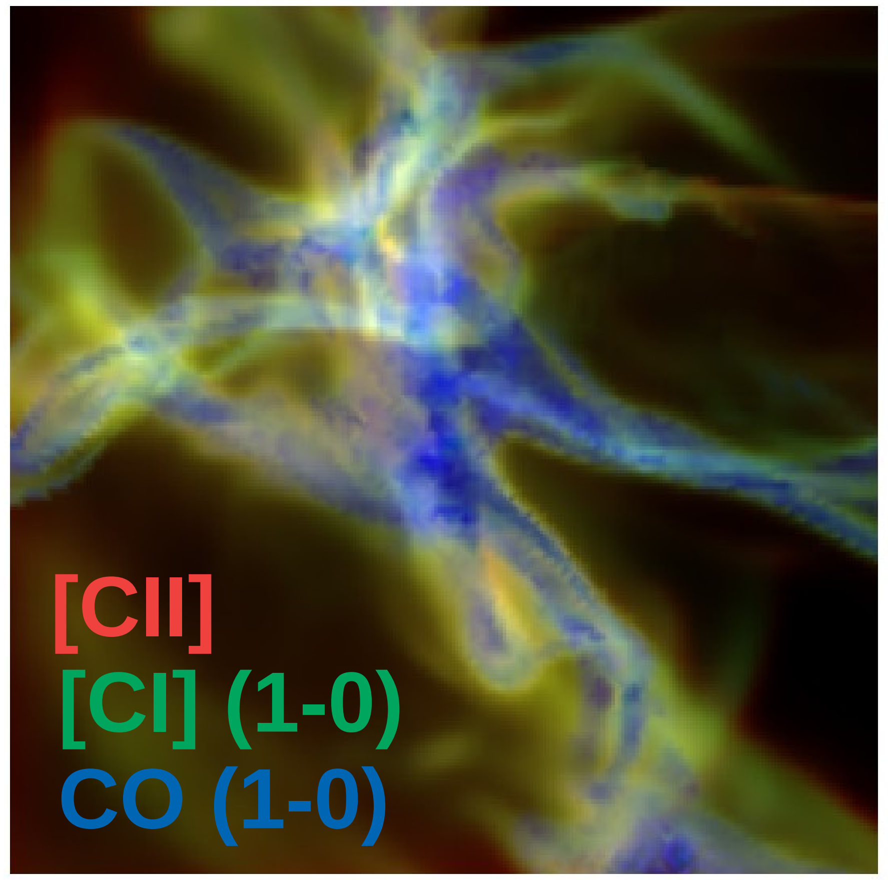


Cooling functions (Λ)

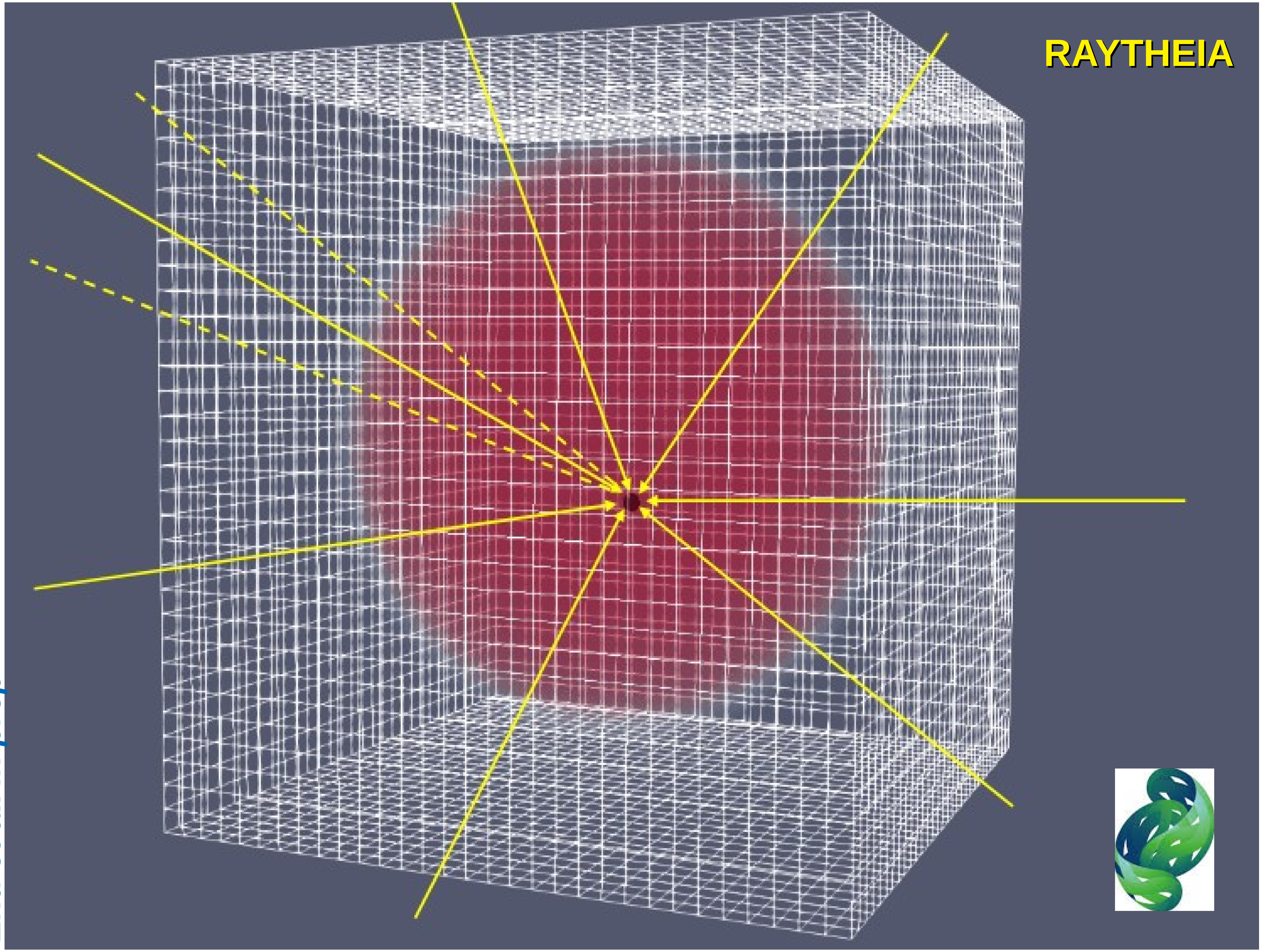
- Line emission
- Dust grain emission (SED)
- Molecular rotational and vibrational transitions (SLED)



[CII] [CI](1-0) CO (1-0)

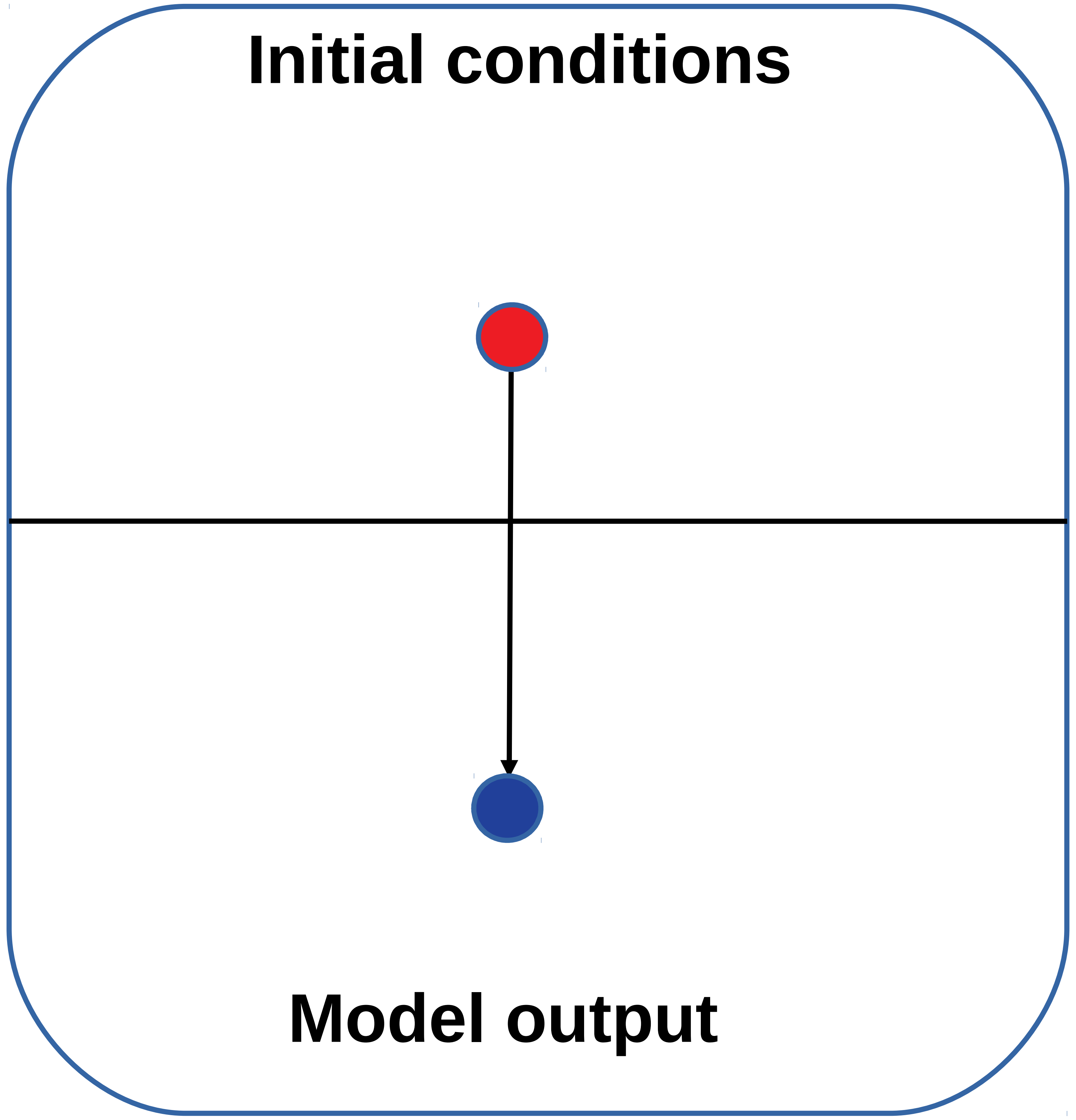


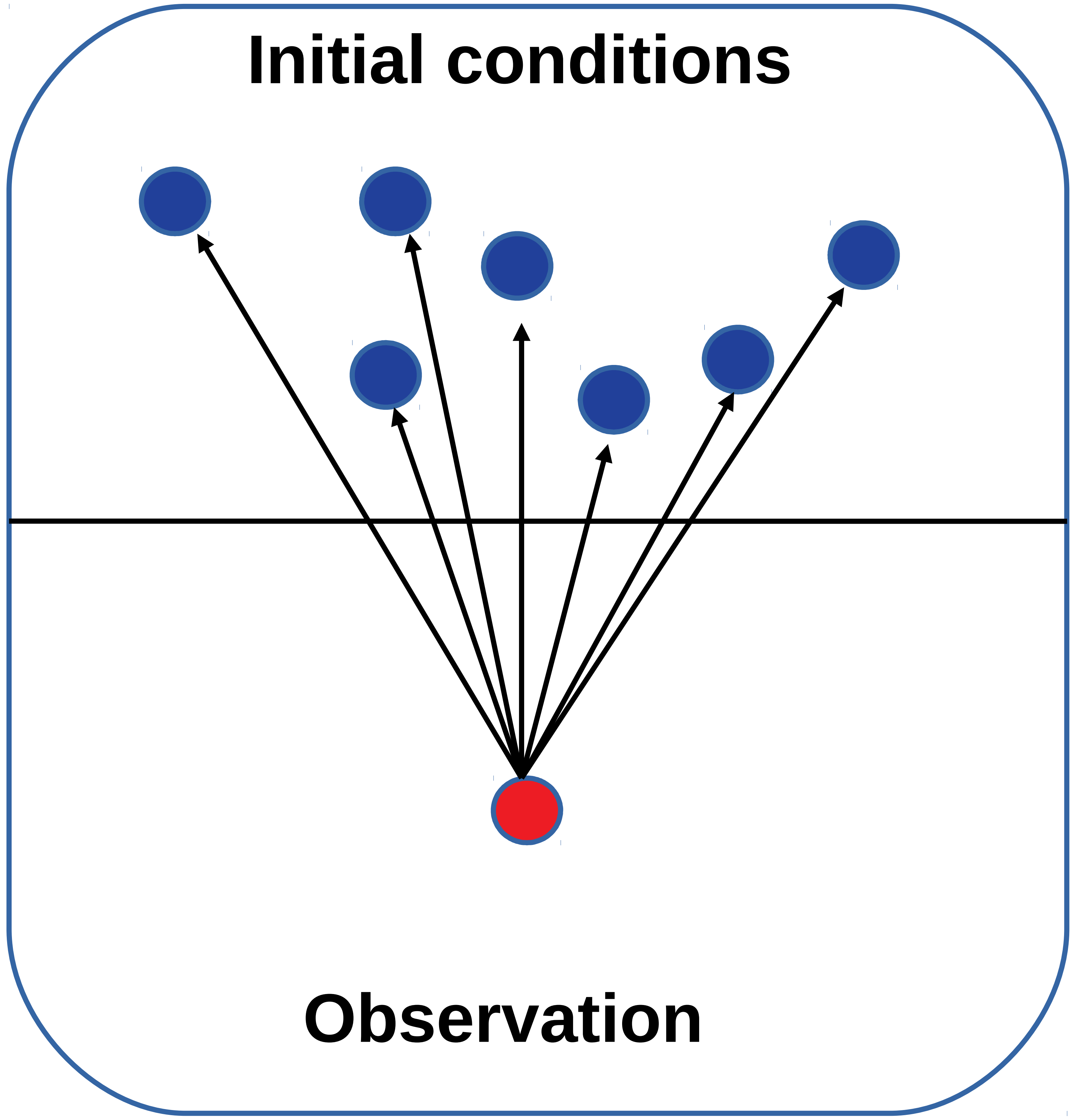
The 3D-PDR code (Bisbas+ 2012; Zhu+ *in prep*)



Zhu et al. *in prep*

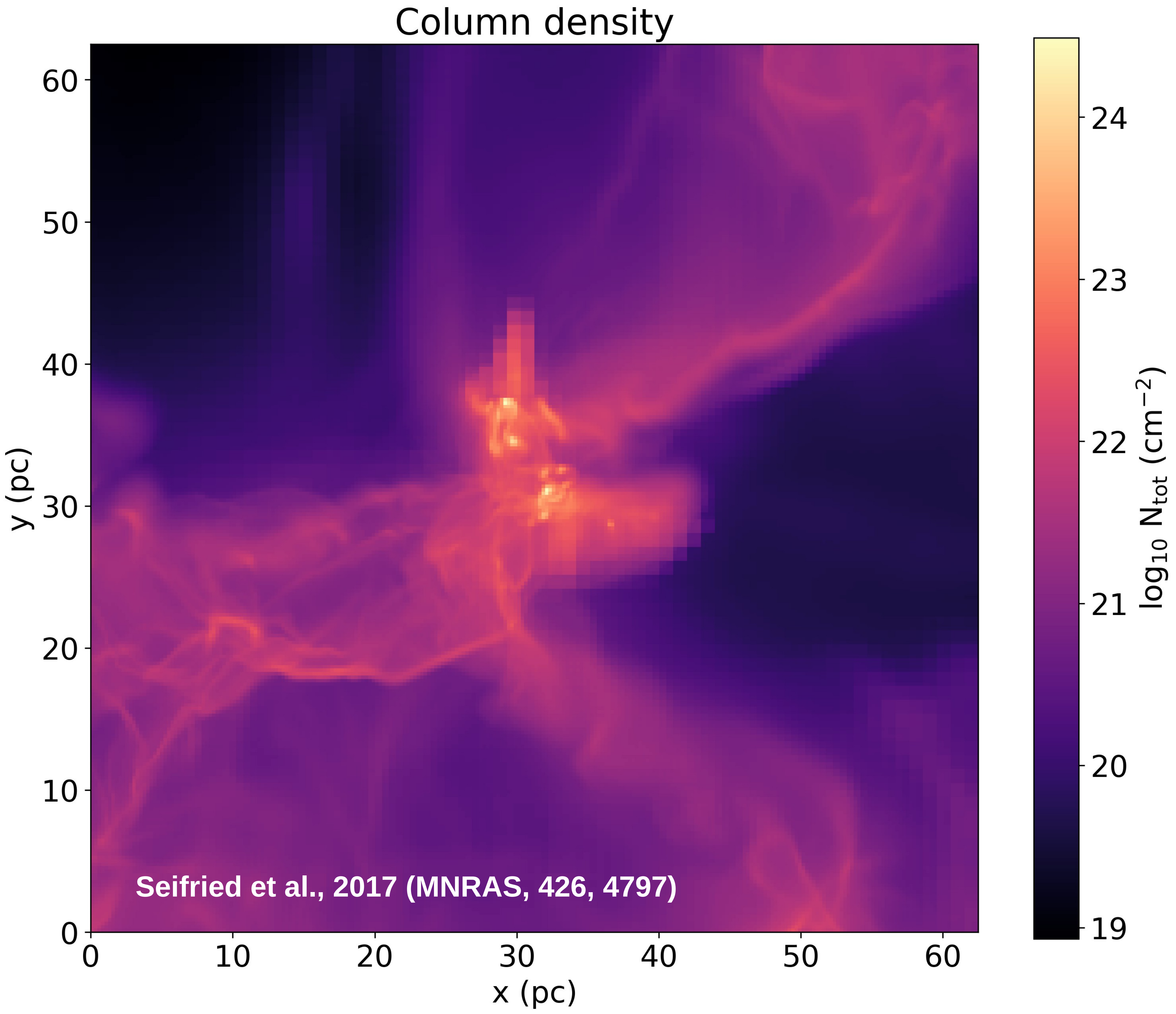
Connecting models with observations





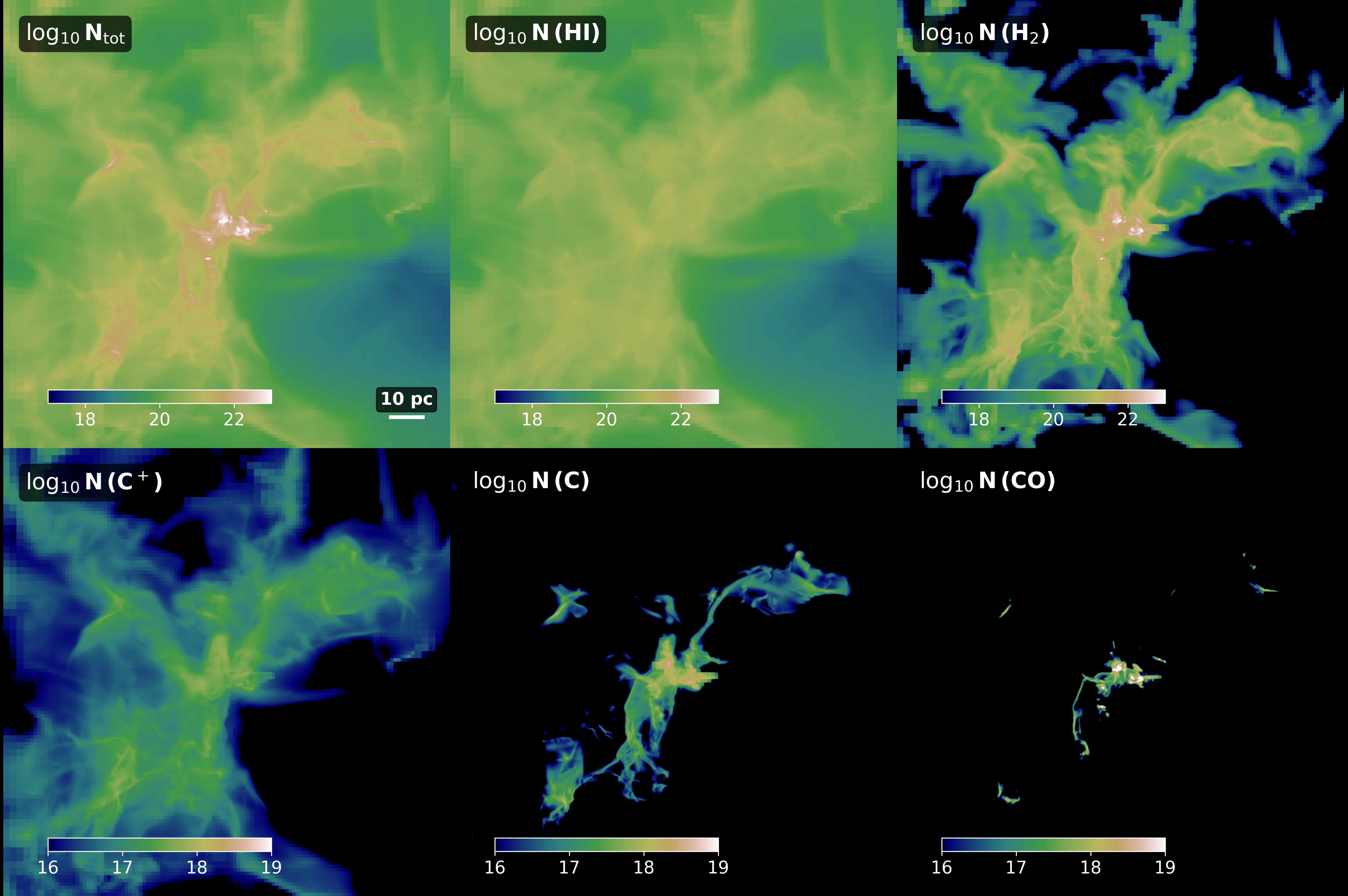
Linking observations with models is not trivial

Modelling the PDR of a star-forming region (Seifried+ 2017)

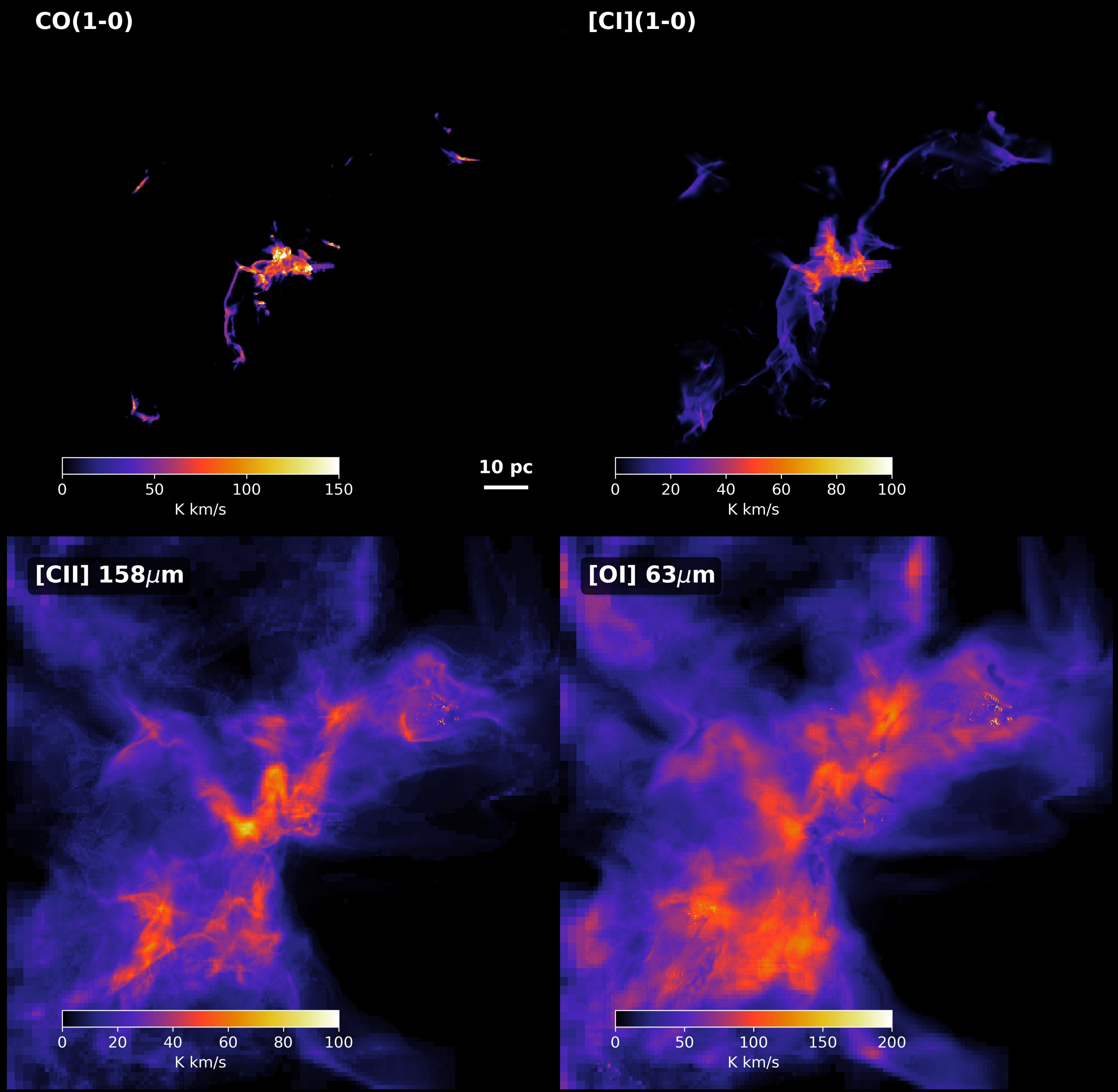


- SILCC models (Cologne group)
- Molecular cloud formation (2 clouds)
- Full extent of 125 pc
- Resolution of 512^3 (0.24pc resolution)
- Hydro + Self-gravity

Highest resolution PDR model to date!
Zhu et al. *in prep.*

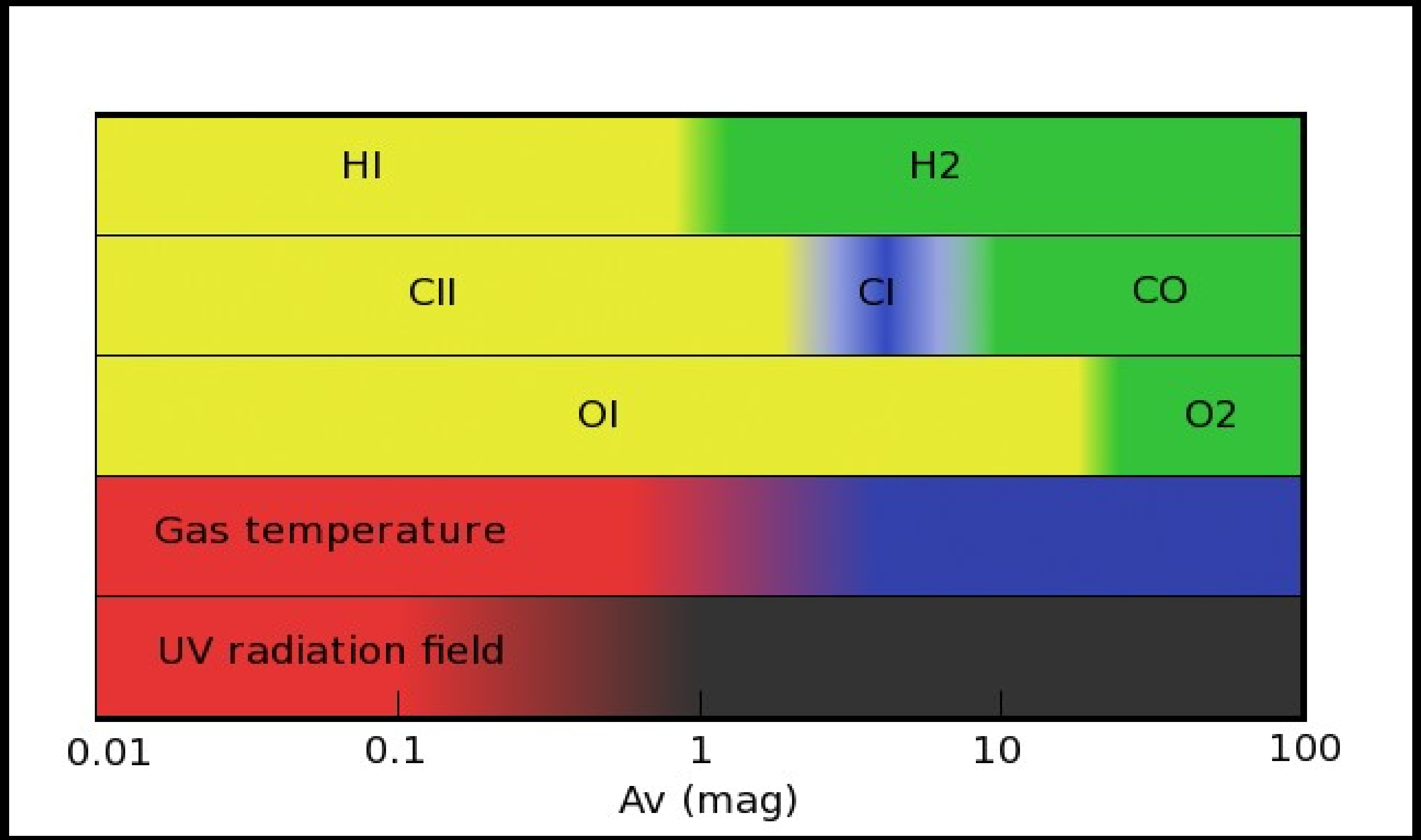


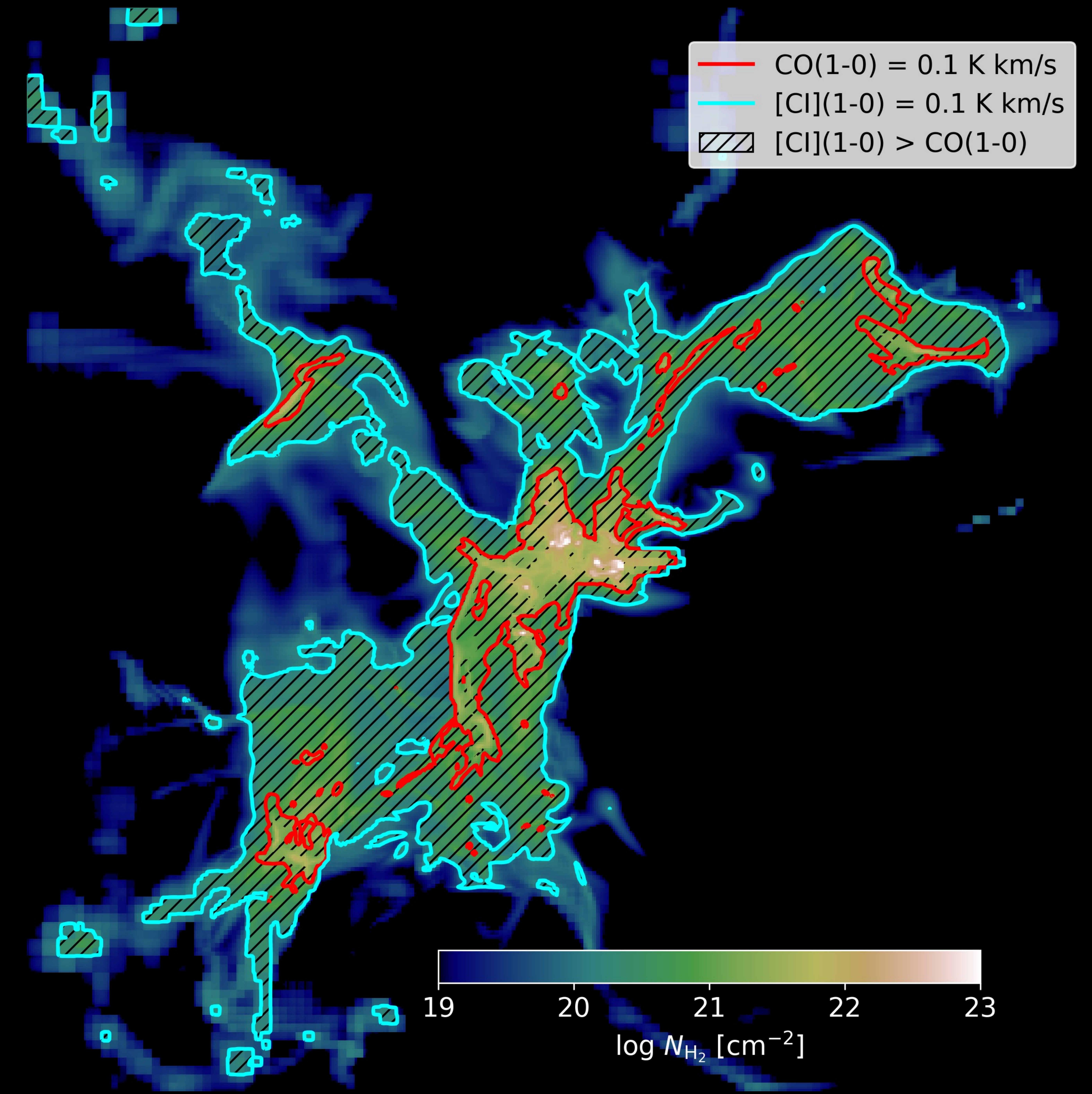
$\log_{10}$ N$_{tot}$
18
20
22
10 pc
$\log_{10}$ N (HI)
18
20
22
$\log_{10}$ N (H$_2$)
18
20
22
$\log_{10}$ N (C$^+$)
16
17
18
19
$\log_{10}$ N (C)
16
17
18
19
$\log_{10}$ N (CO)
16
17
18
19



Carbon cycle (CII / CI / CO)

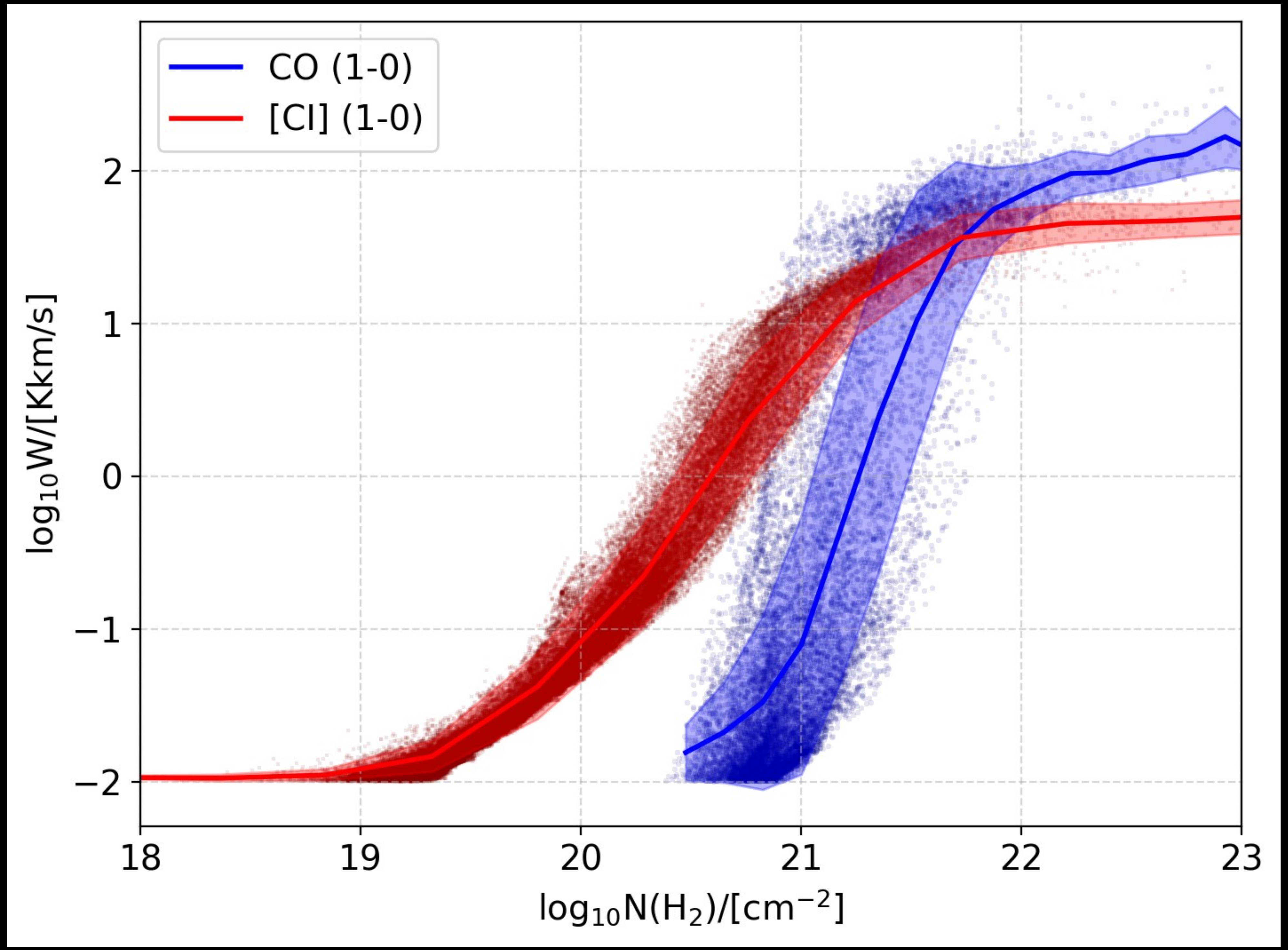
Calculated X-factor = **2.3e20 cm^{-2}/(K km/s)** matching with observations (2e20 cm^{-2}/(K km/s) ±30%, Bolatto+13)

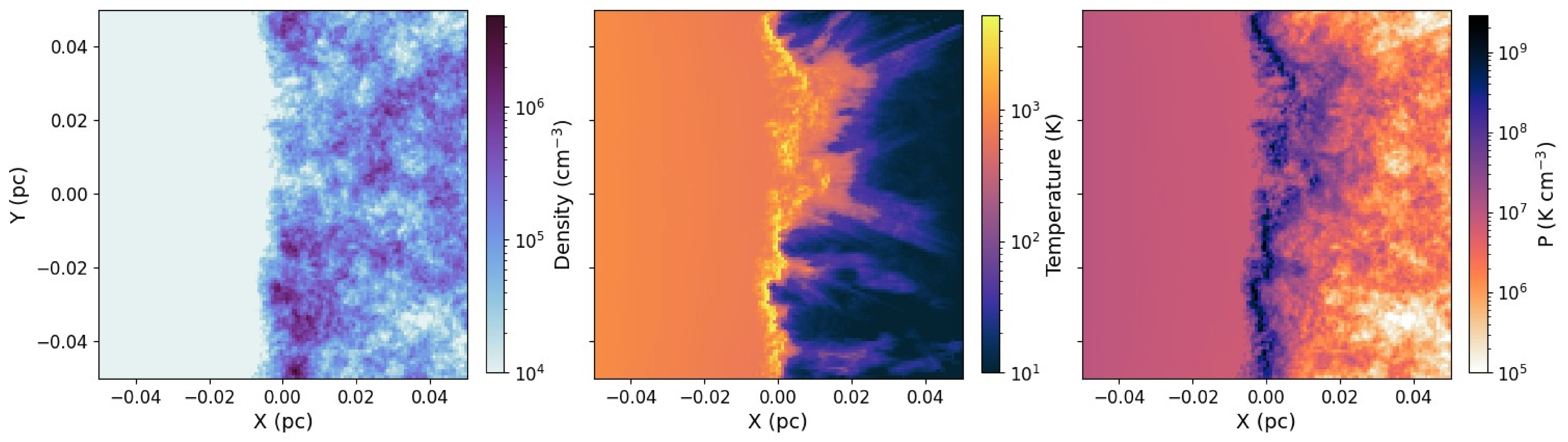




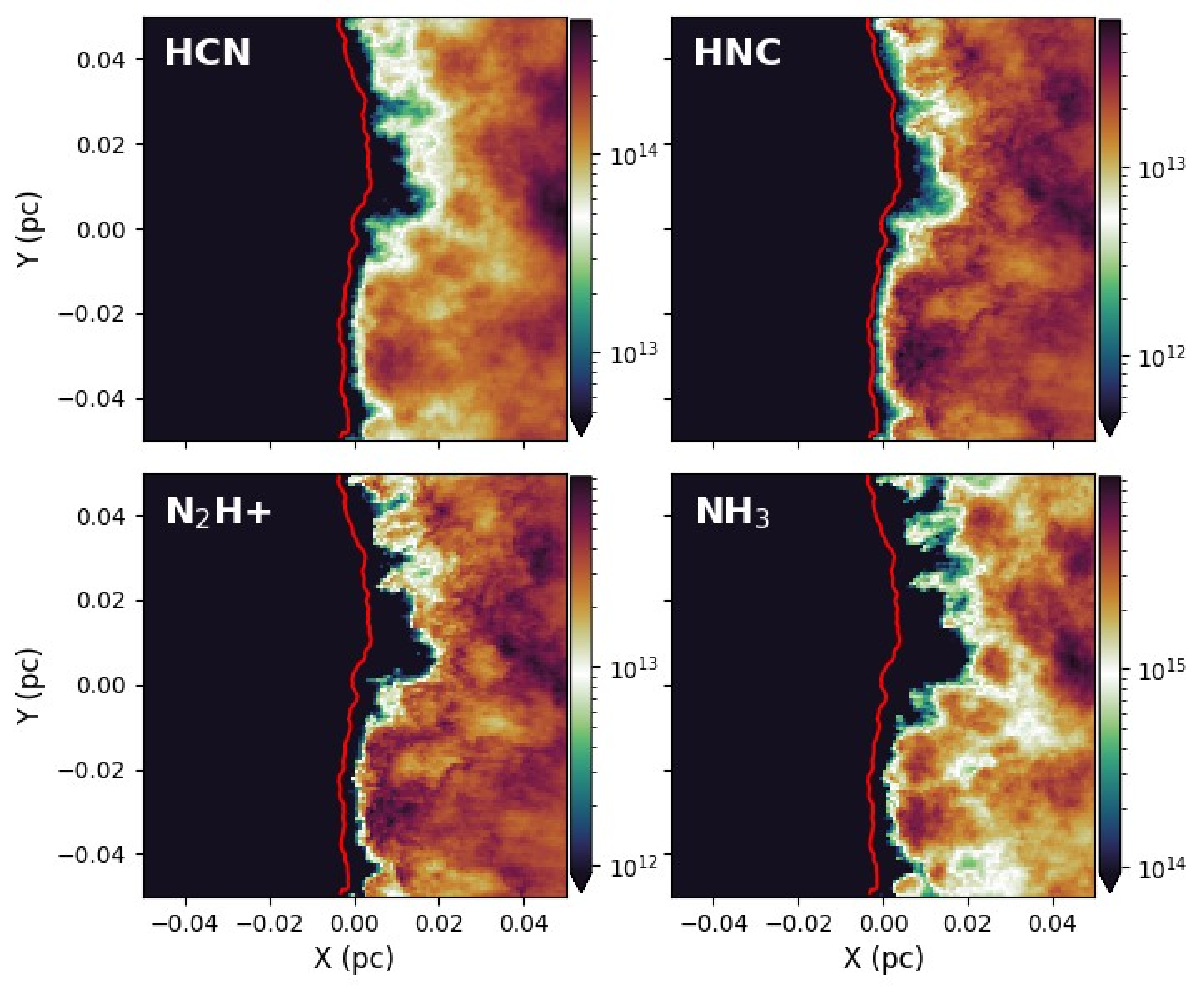
`CO-dark' gas (van Dishoeck 1992)

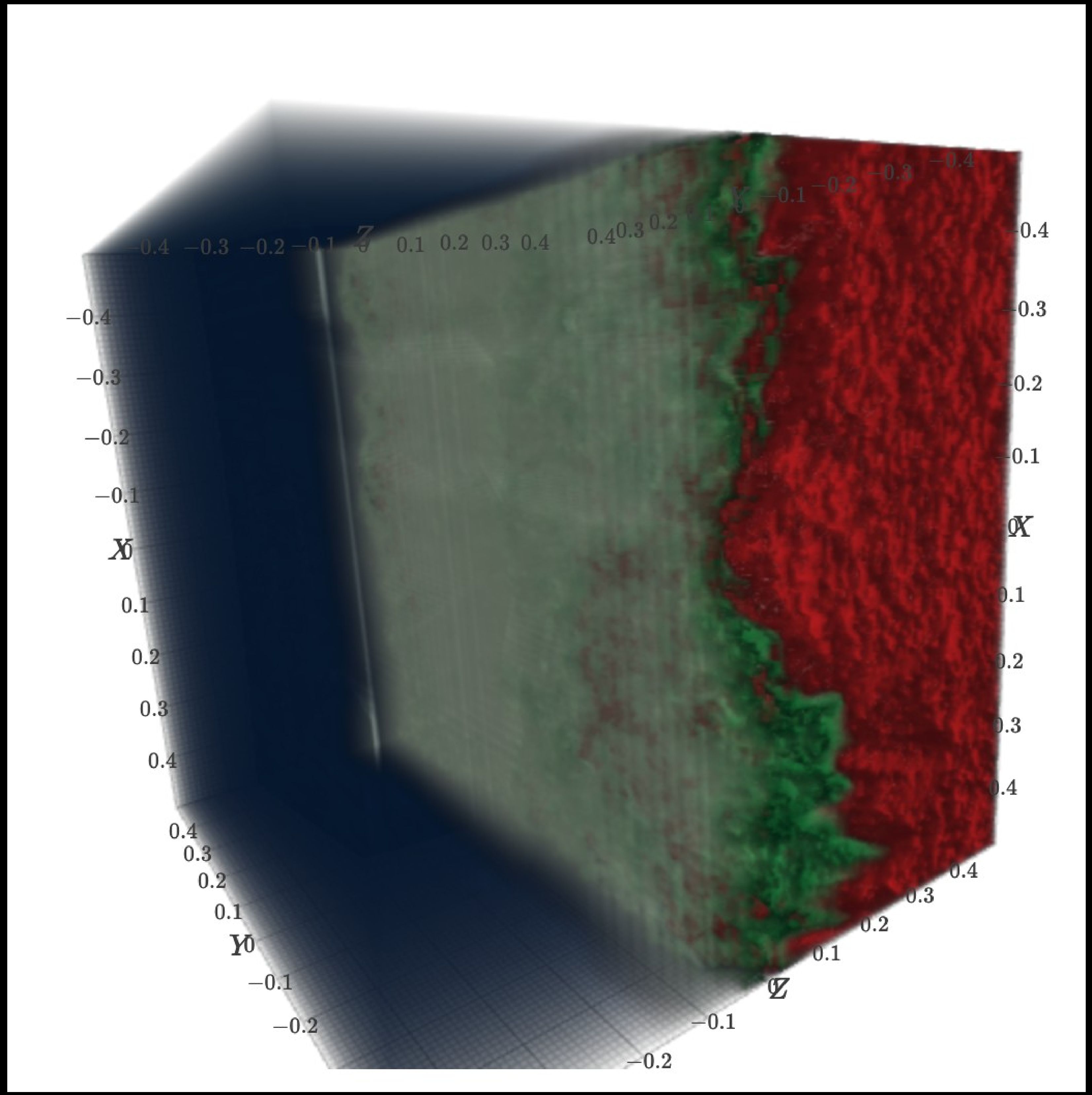
>95% of NH_2 observed with [CI] (1-0)
~65% of NH_2 observed with CO(1-0)
In agreement with observations (e.g. Lo+ 14; Jiao+ 17, 19, 21; Crocker+ 19)



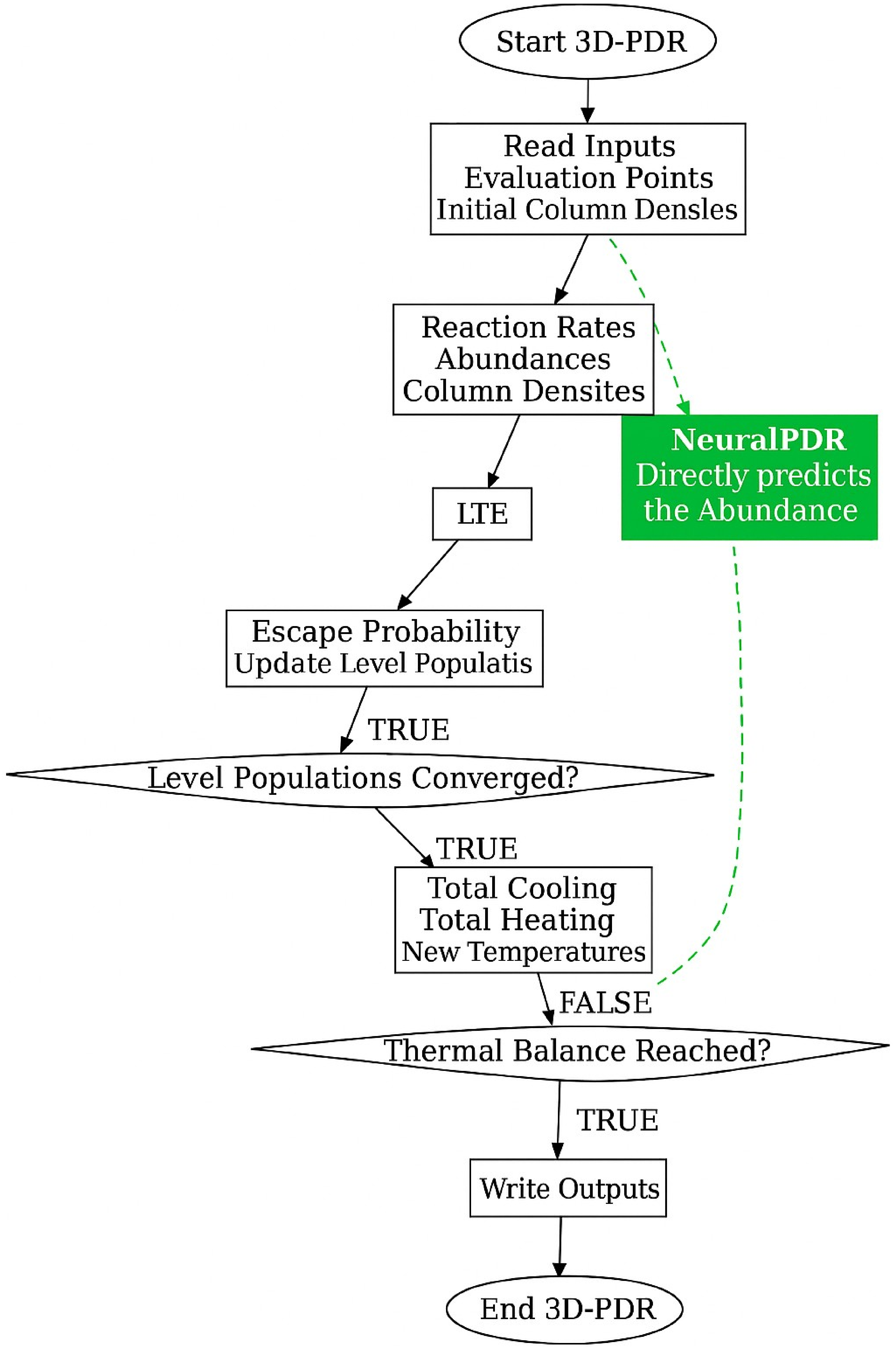


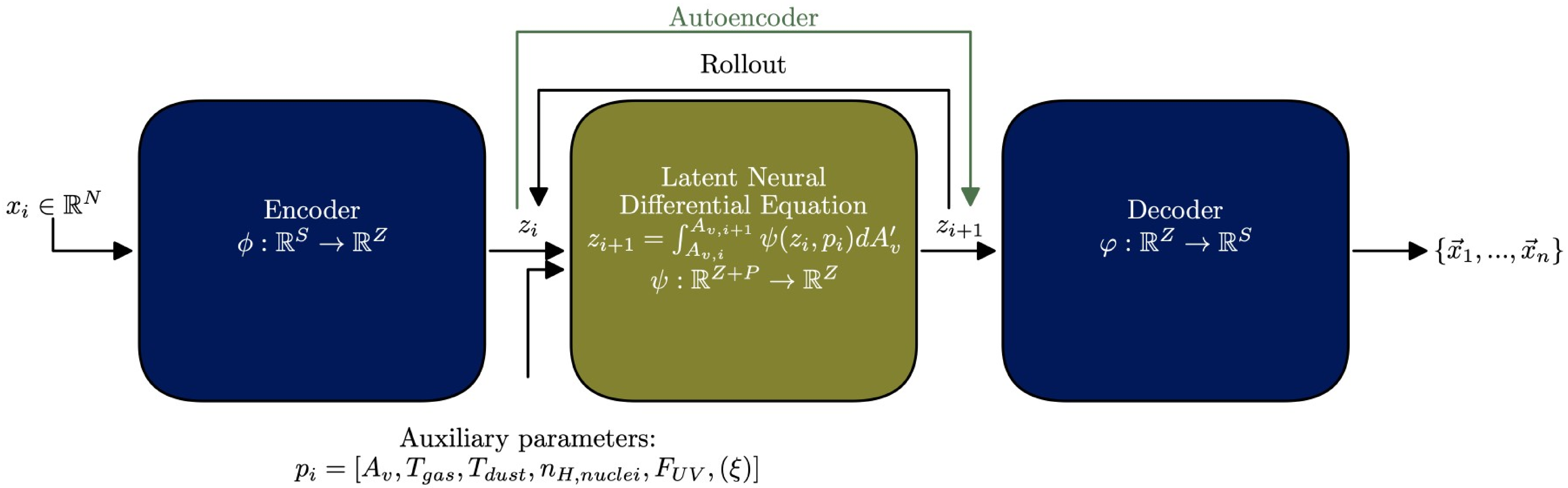
Models by B. Gaches
(Duisburg-Essen, Germany)





Using ML to speed-up the calculations (Tang+ *in prep*)





Concept: use neural networks to compress, evolve and decompress chemical time series

Vermarien+ 24, 25

3DPDR
- simulated data

Generate dataset
- ML.dat→HDF5

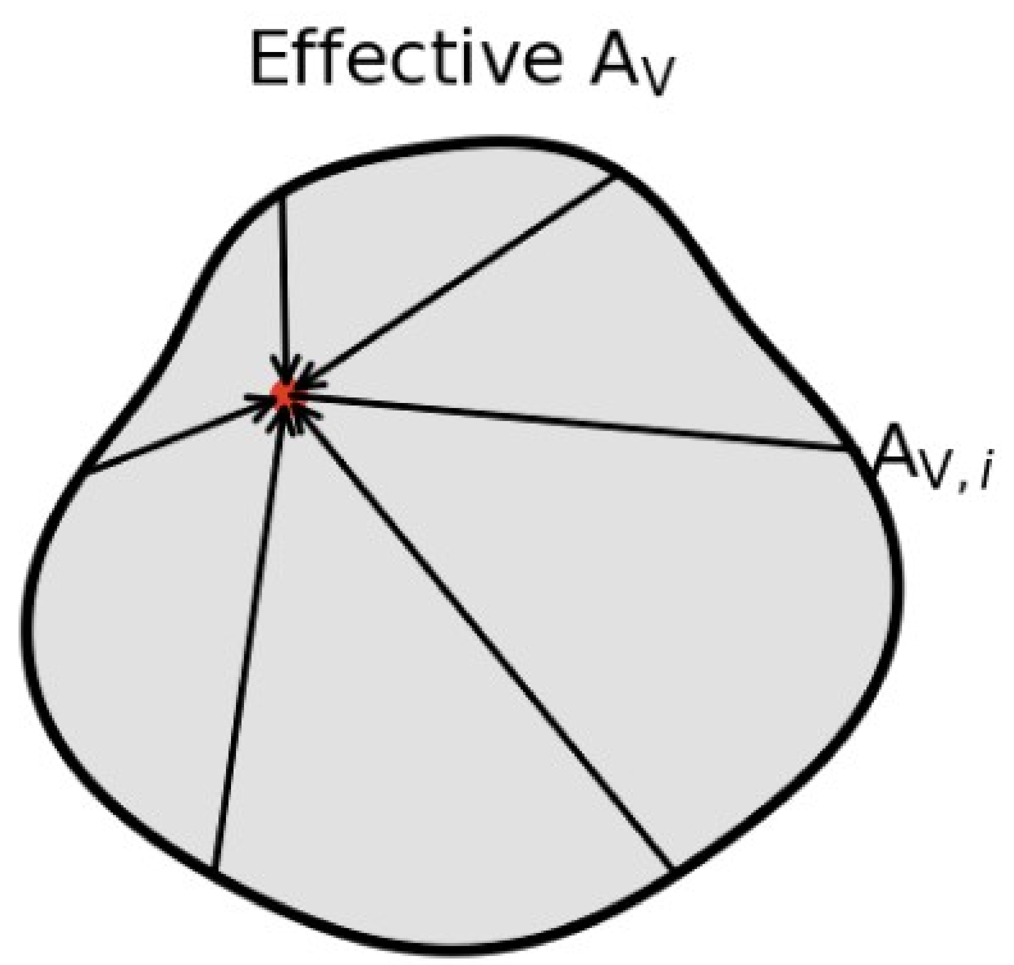
NerualPDR
- Train and Inference

Column density
- Integrate along the z-axis →2D

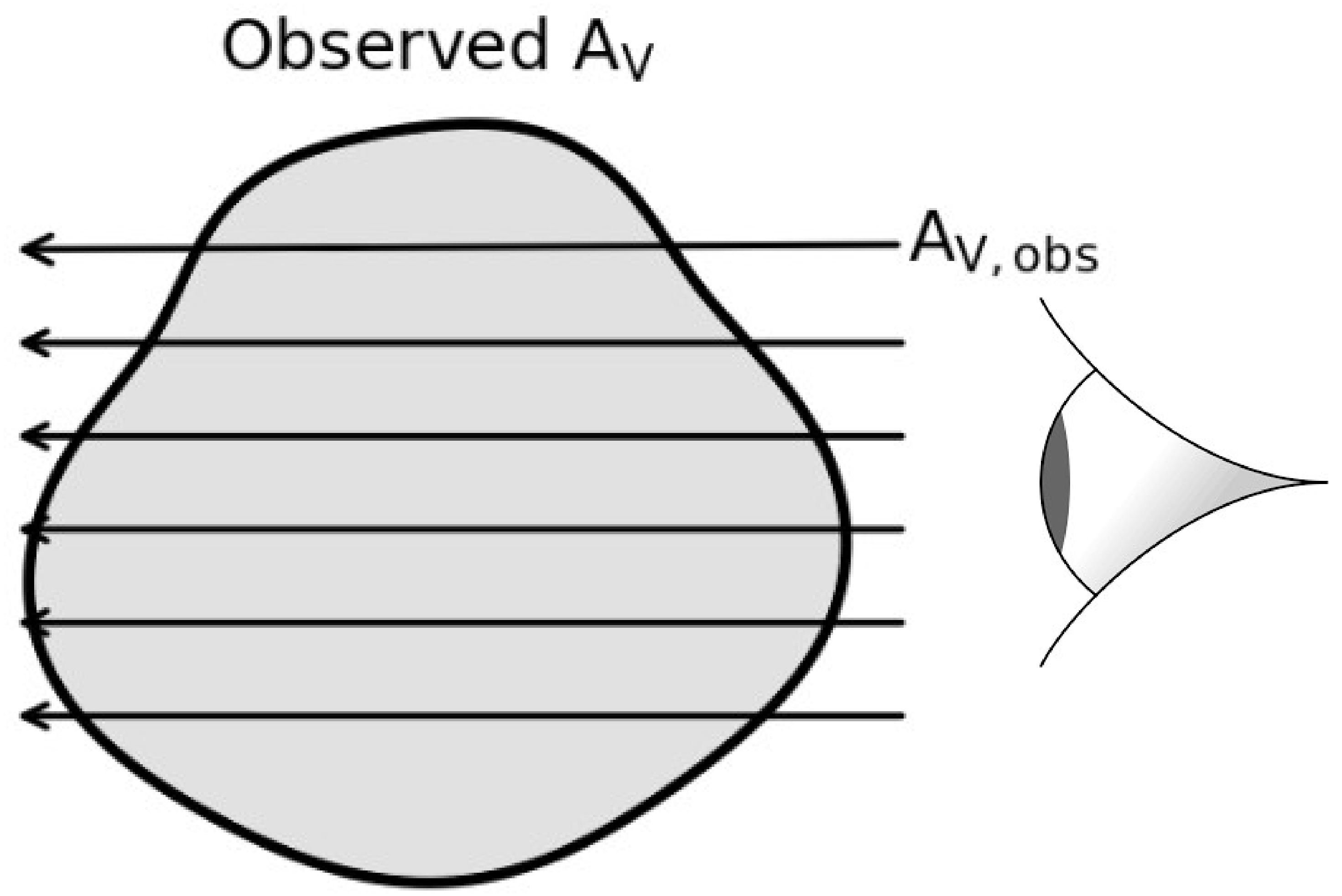
Error plot
- True value VS Predict value

Problems in using ML in PDR studies

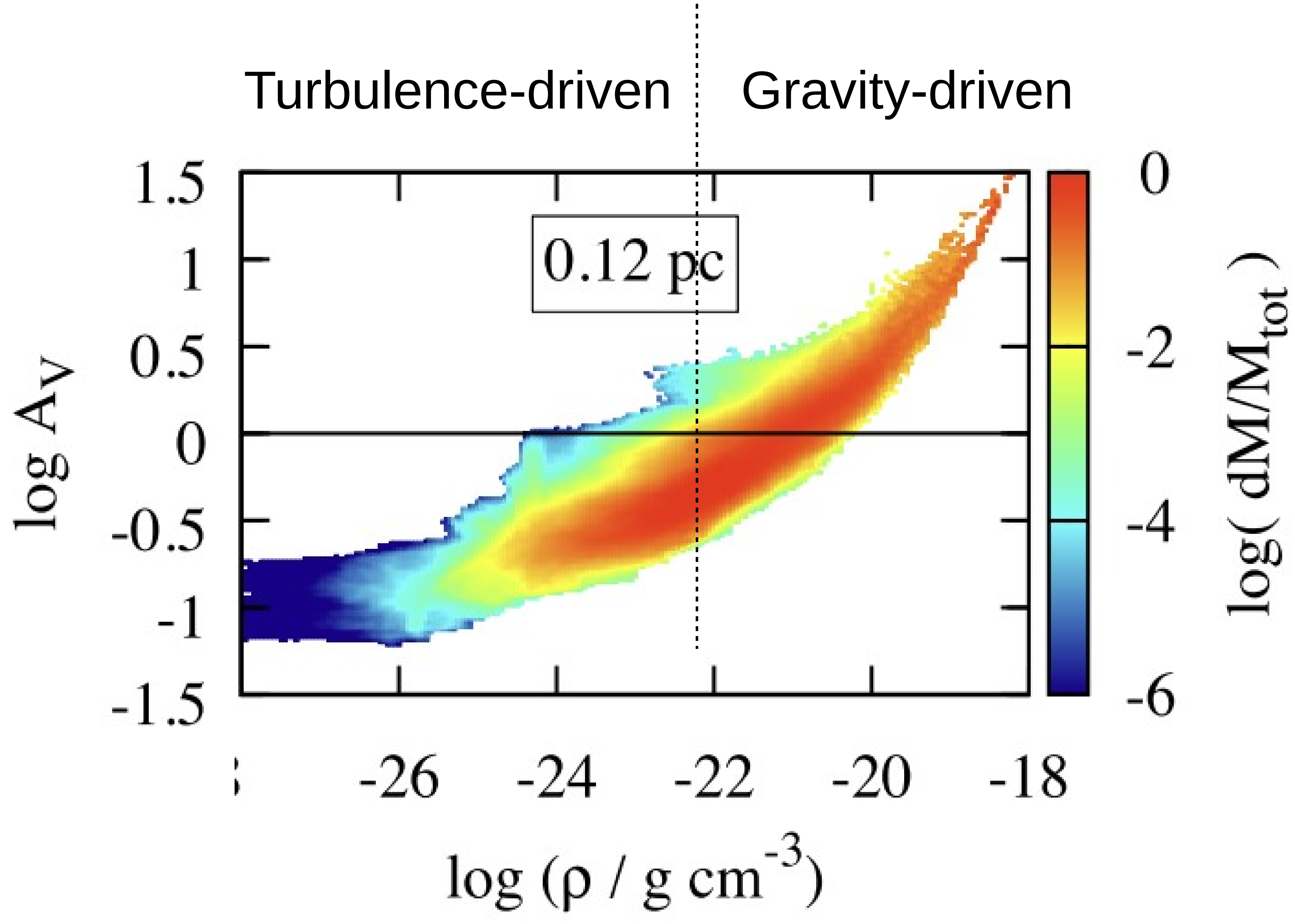
- Generating the training set in 3D is demanding!
- Av,eff – nH relationship



PDR chemistry is controlled by this visual extinction.



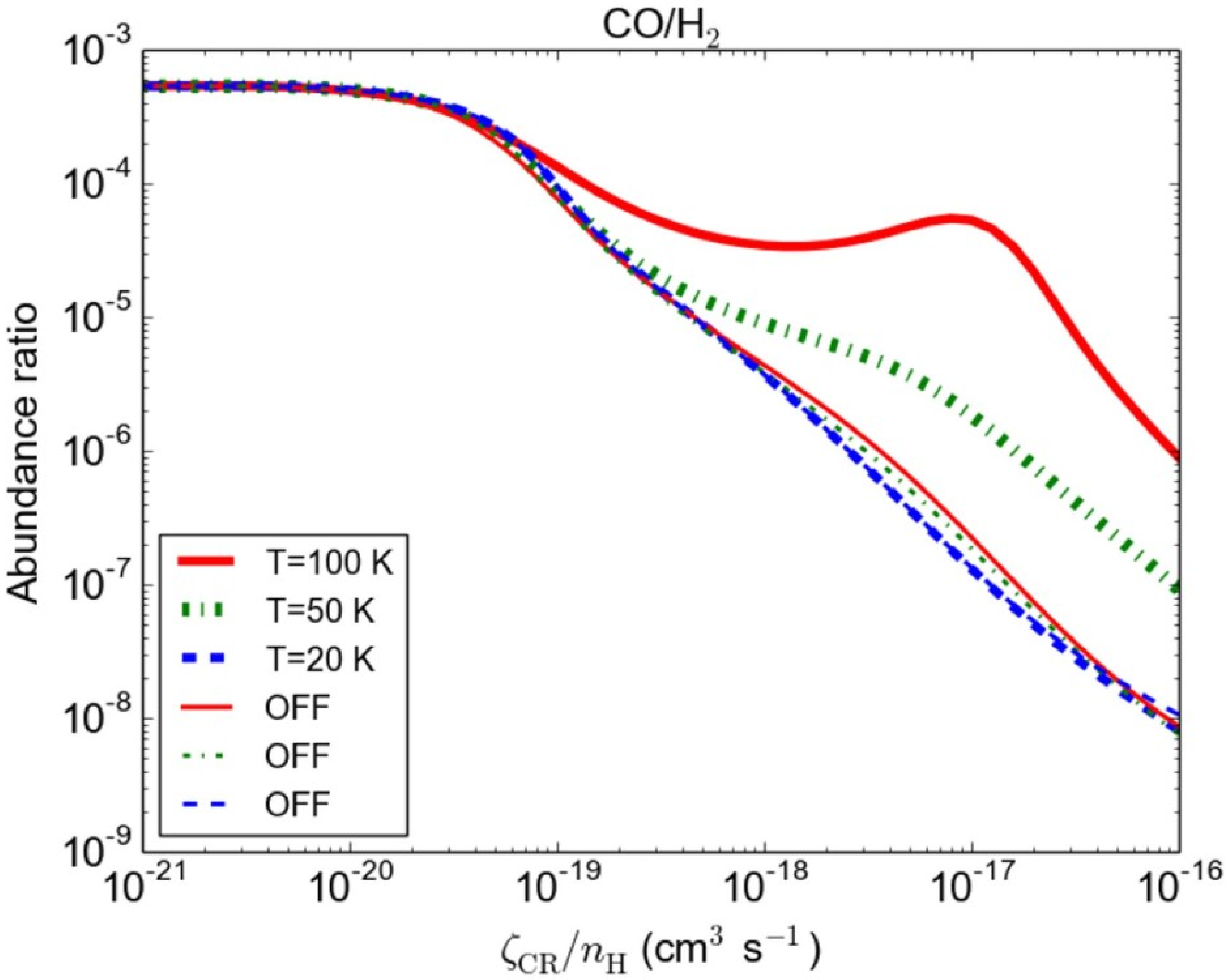
When column-density PDFs are shown, they all use this visual extinction.



Example of Av,eff – nH from a hydrodynamical model (Seifried+ 17)

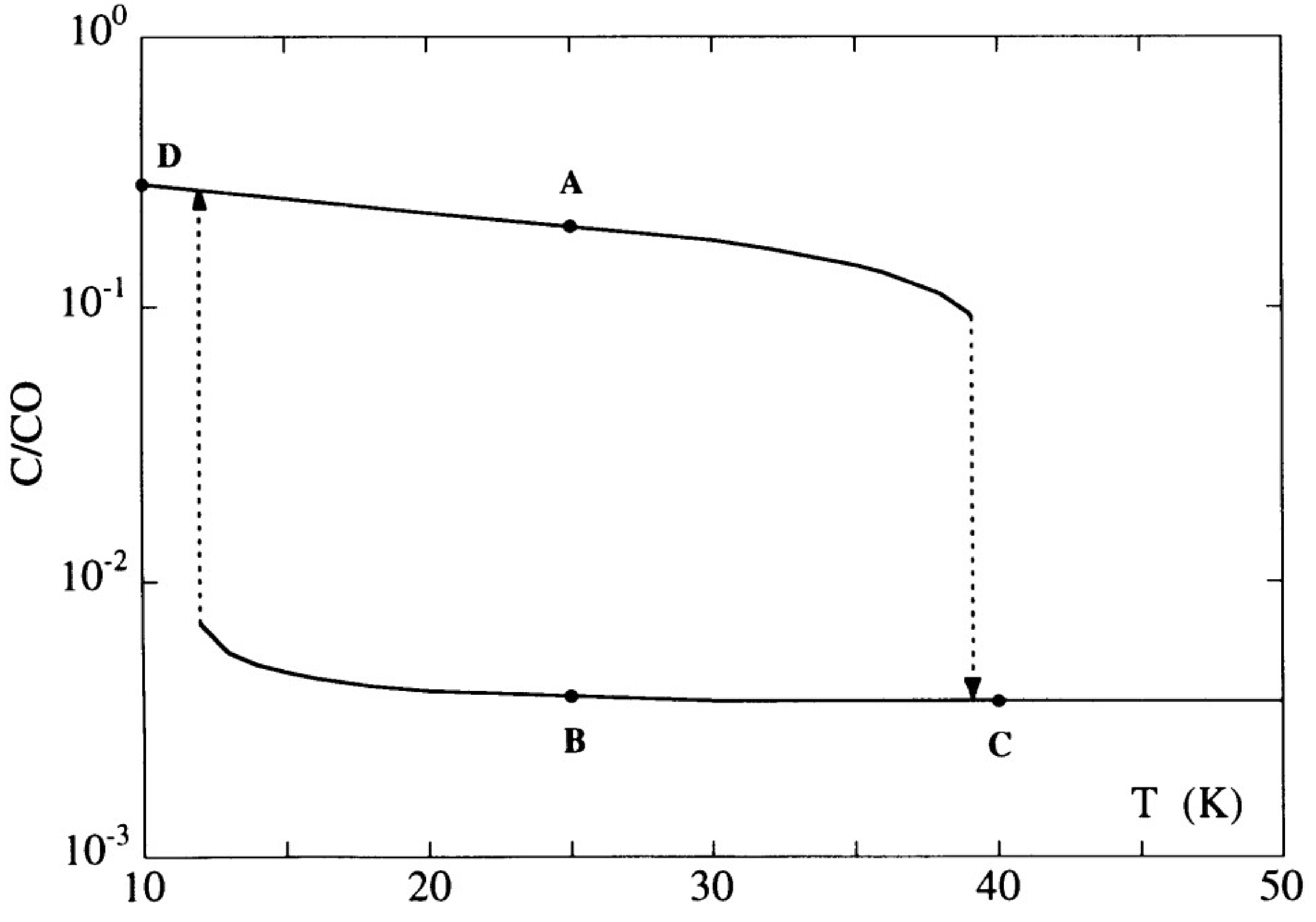
Problems in using ML in PDR studies

- Generating the training set in 3D is demanding!
- Av,eff – nH relationship
- Highly non-linear ODEs

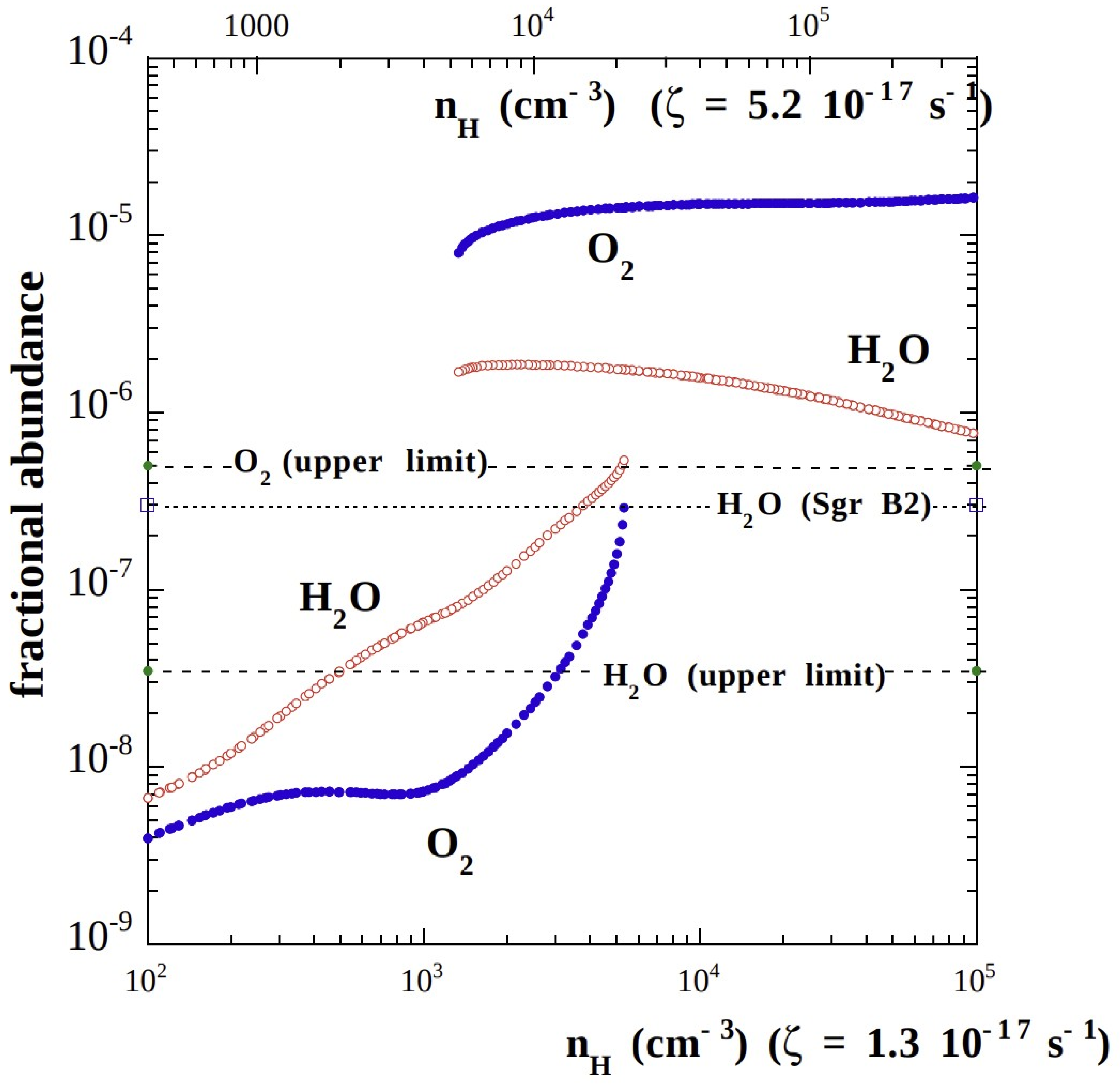


Problems in using ML in PDR studies

- Generating the training set in 3D is demanding!
- Av,eff – nH relationship
- Highly non-linear ODEs
- Bi-stability / non-stable solutions



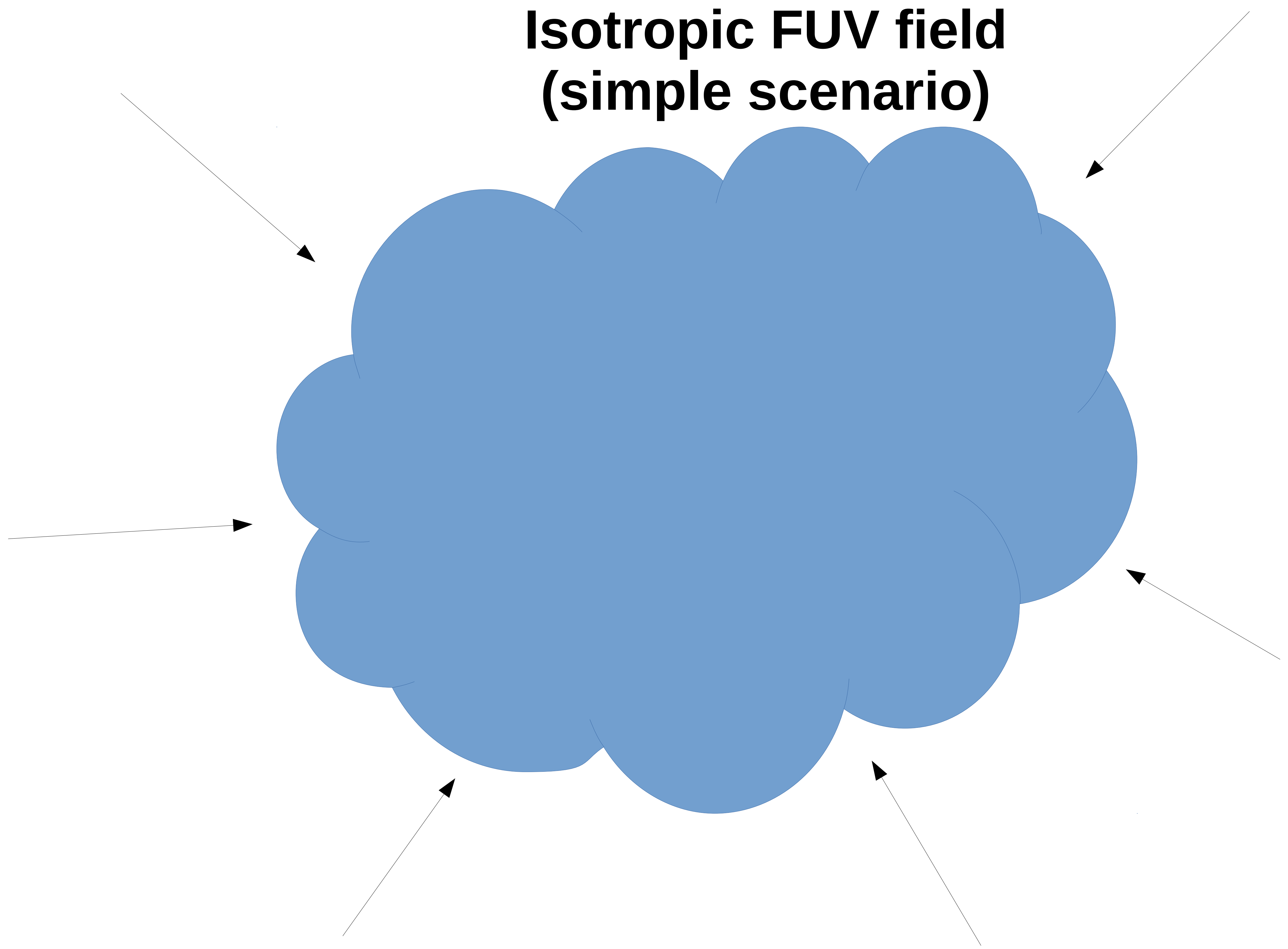
Le Bourlot+ (1993)

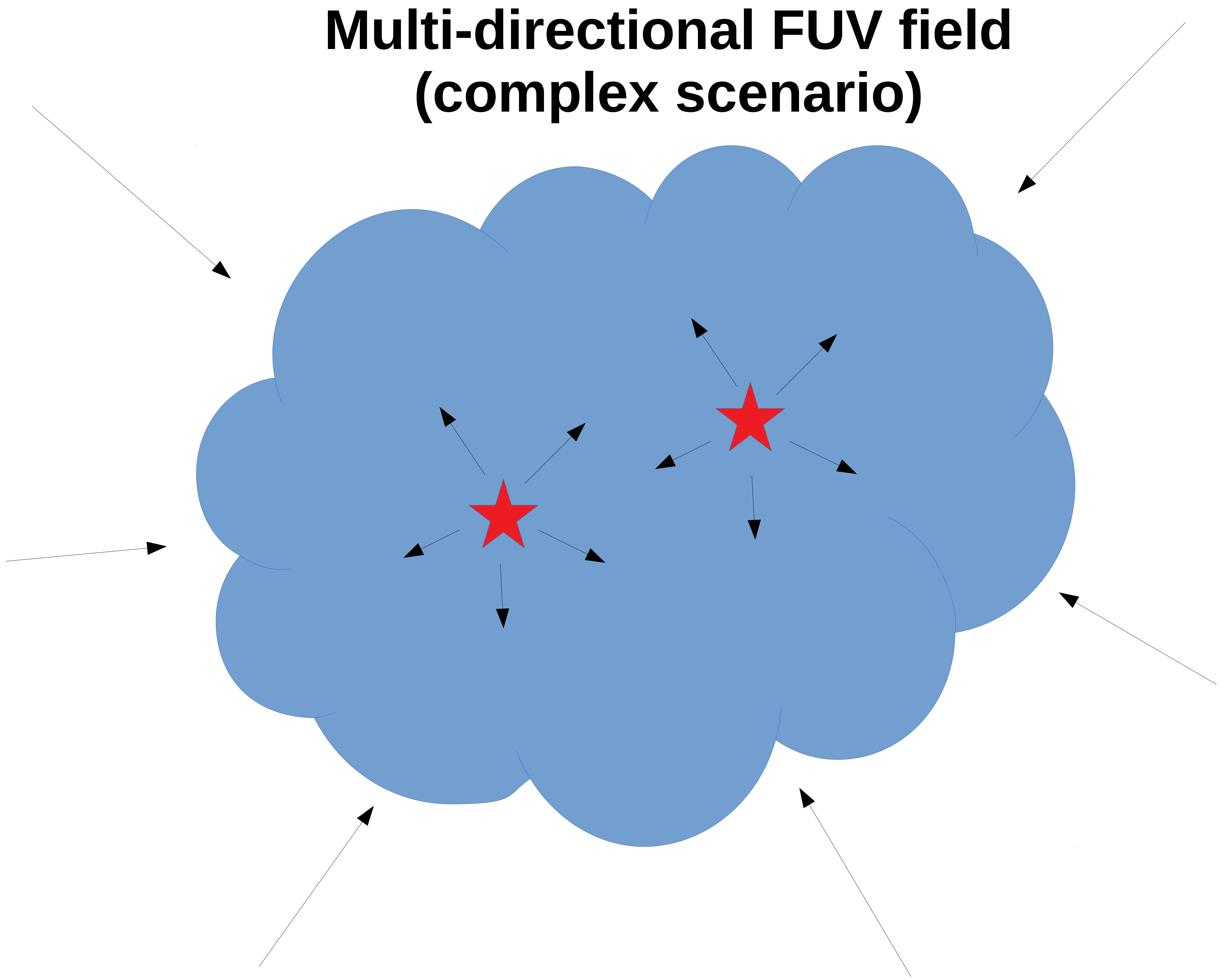


Viti+ (2001)

Problems in using ML in PDR studies

- Generating the training set in 3D is demanding!
- Av,eff – nH relationship
- Highly non-linear ODEs
- Bi-stability / non-stable solutions
- Multi-directional FUV field





Conclusions and remarks

- Modelling PDRs in 3D captures inhomogenities.

- Training ML-modules for on-the-fly 3D PDR calculations remains a challenge, primarily due to the high-computational cost required.

- ML can accelerate PDR calculations by providing the most appropriate initial guesses for the thermal balance iterations.

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