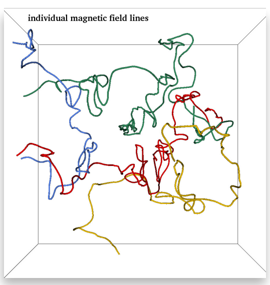
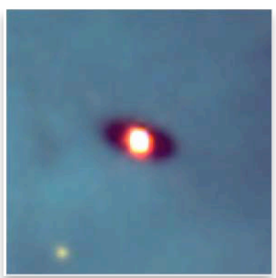
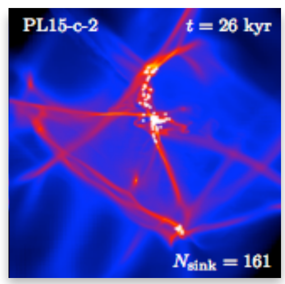
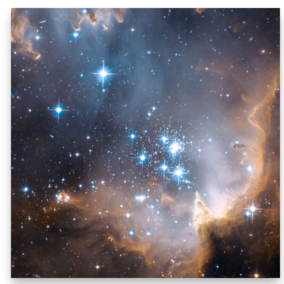
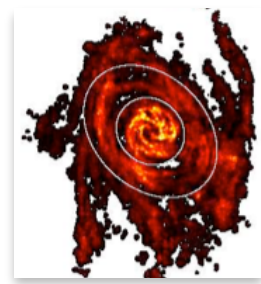
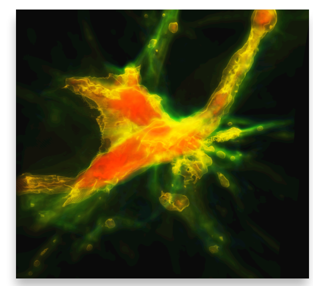
ISM Dynamics and Star Formation



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Institut für Theoretische Astrophysik

thanks to ...

... people in the star formation group at Heidelberg University:

Christian Baczynski, Erik Bertram, Frank Bigiel, Andre Bubel, Diane Cormier, Volker Gaibler, Simon Glover, Dimitrious Gouliermis, Tilman Hartwig, Juan Ibanez, Christoph Klein, Lukas Konstandin, Mei Sasaki, Jennifer Schober, Rahul Shetty, Rowan Smith, László Szűcs

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... many collaborators abroad!

Deutsche Forschungsgemeinschaft DFG

ISM-SPP

BADEN-WÜRTTEMBERG STIFTUNG Wir stiften Zukunft

HGSFP

IMPRS

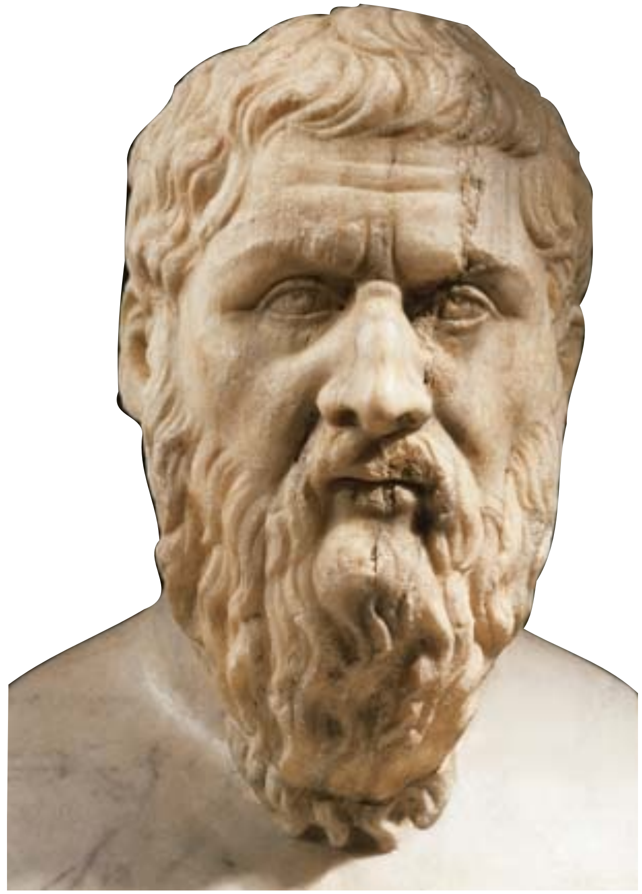
erc European Research Council

agenda

- introductory remarks
  - relation between measurement and underlying physics
- applications / controversies / puzzles
  - global star formation relations
    are we sure we see universal dependencies?
  - molecular gas
    are we sure we see all H_2 gas?
  - filaments
    are they real (ly everywhere)?

NGC 3324 (Hubble, NASA/ESA)

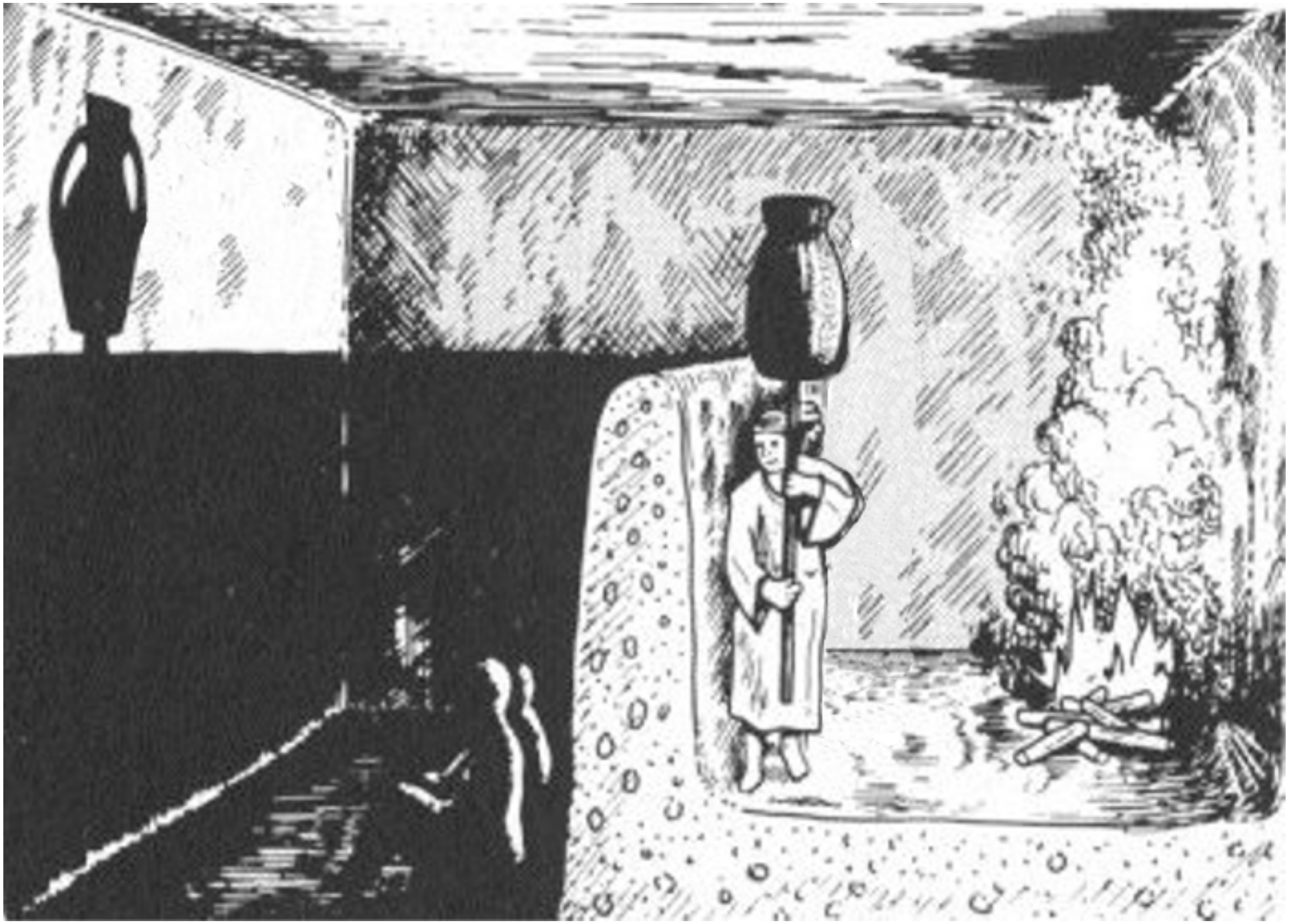
prolegomena



Platon
428/427–348/347 BC

Capitoline Museum, Rome.

Plato's allegory of the cave*

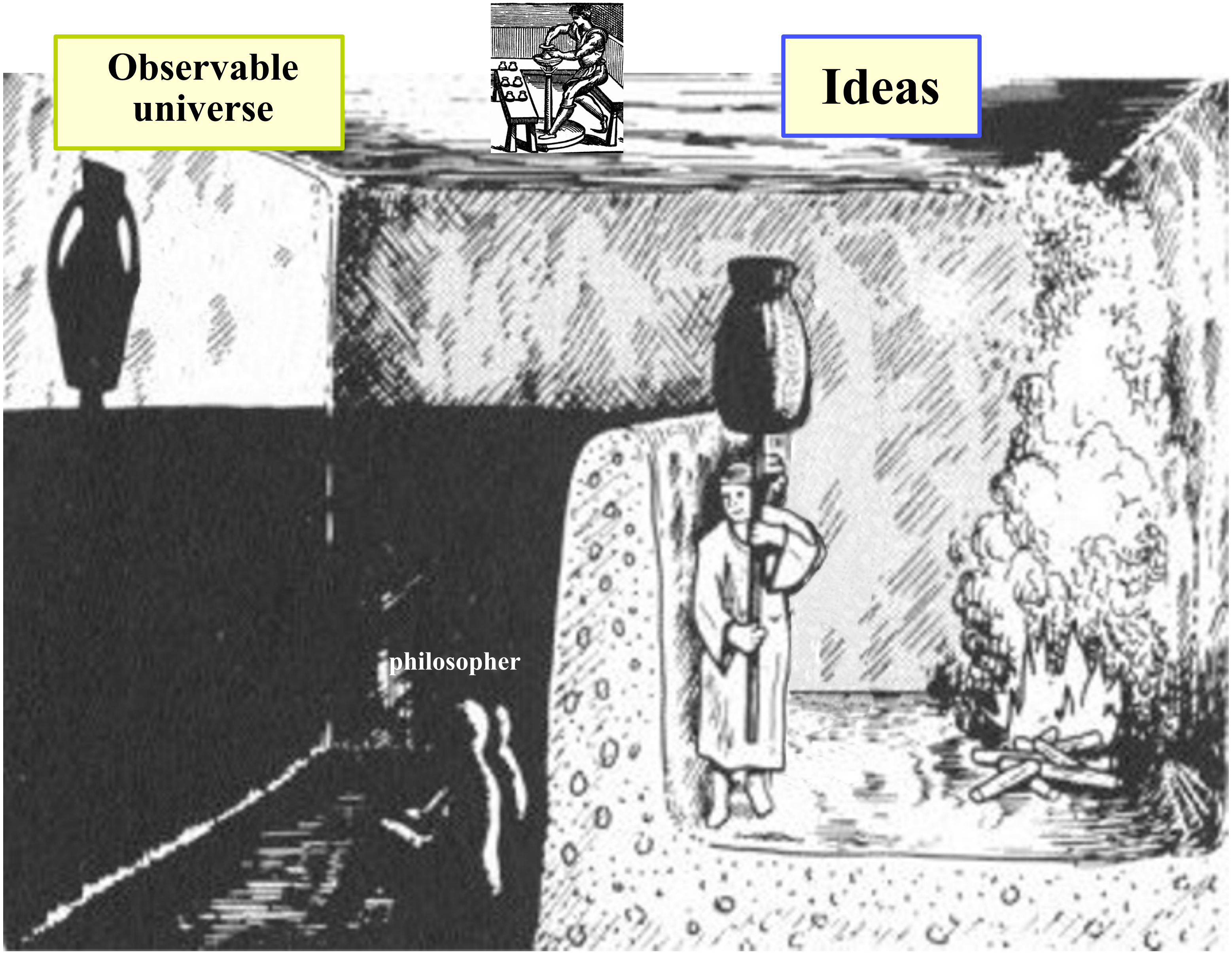


Laszlo Szücs, image from criticalthinking-mc205.wikispaces.com

* The Republic (514a-520a)

Plato's allegory of the cave*

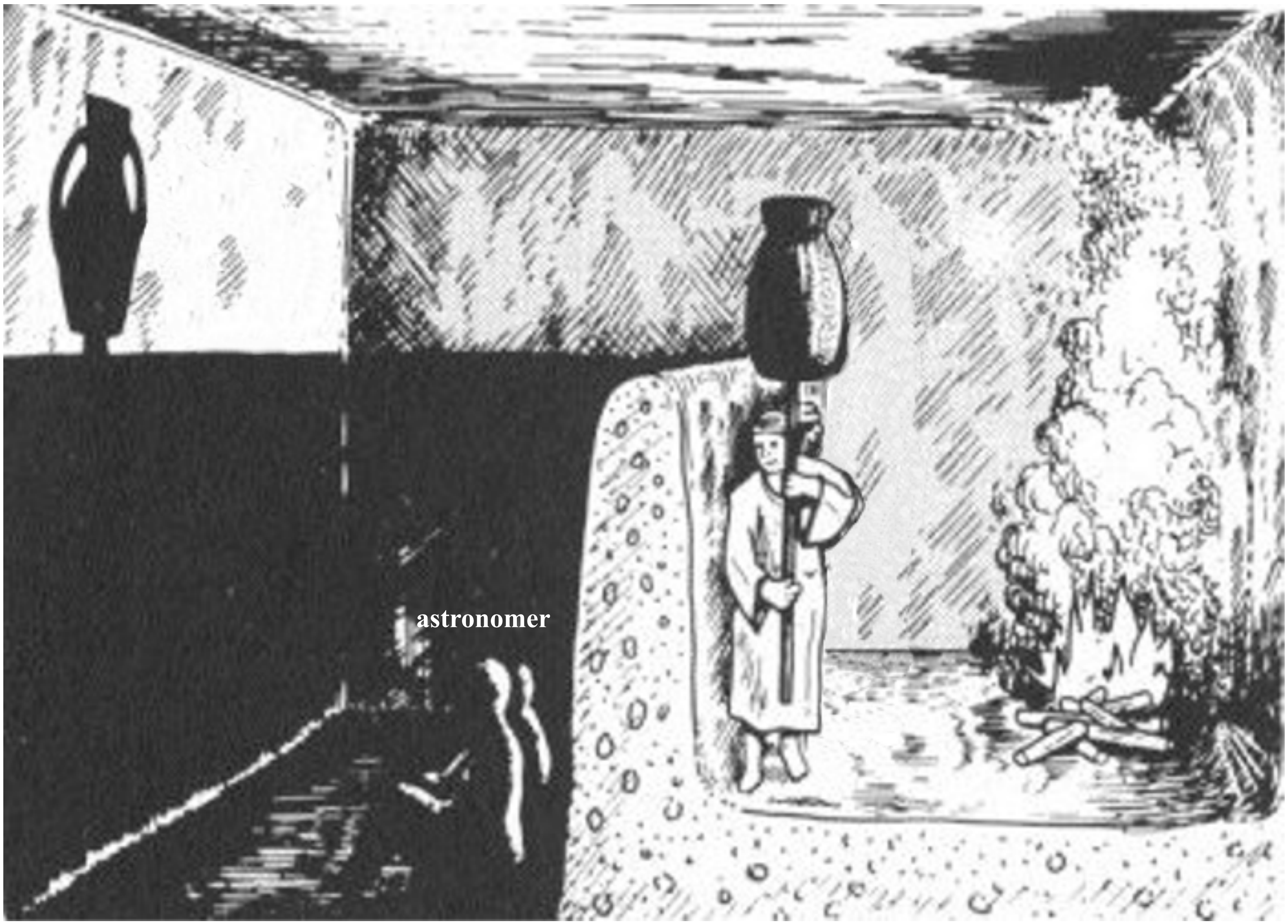
“Demiurge”



Laszlo Szücs, image from criticalthinking-mc205.wikispaces.com

* The Republic (514a-520a)

Plato's allegory of the cave* ↔ Astronomical observations



Laszlo Szücs, image from criticalthinking-mc205.wikispaces.com

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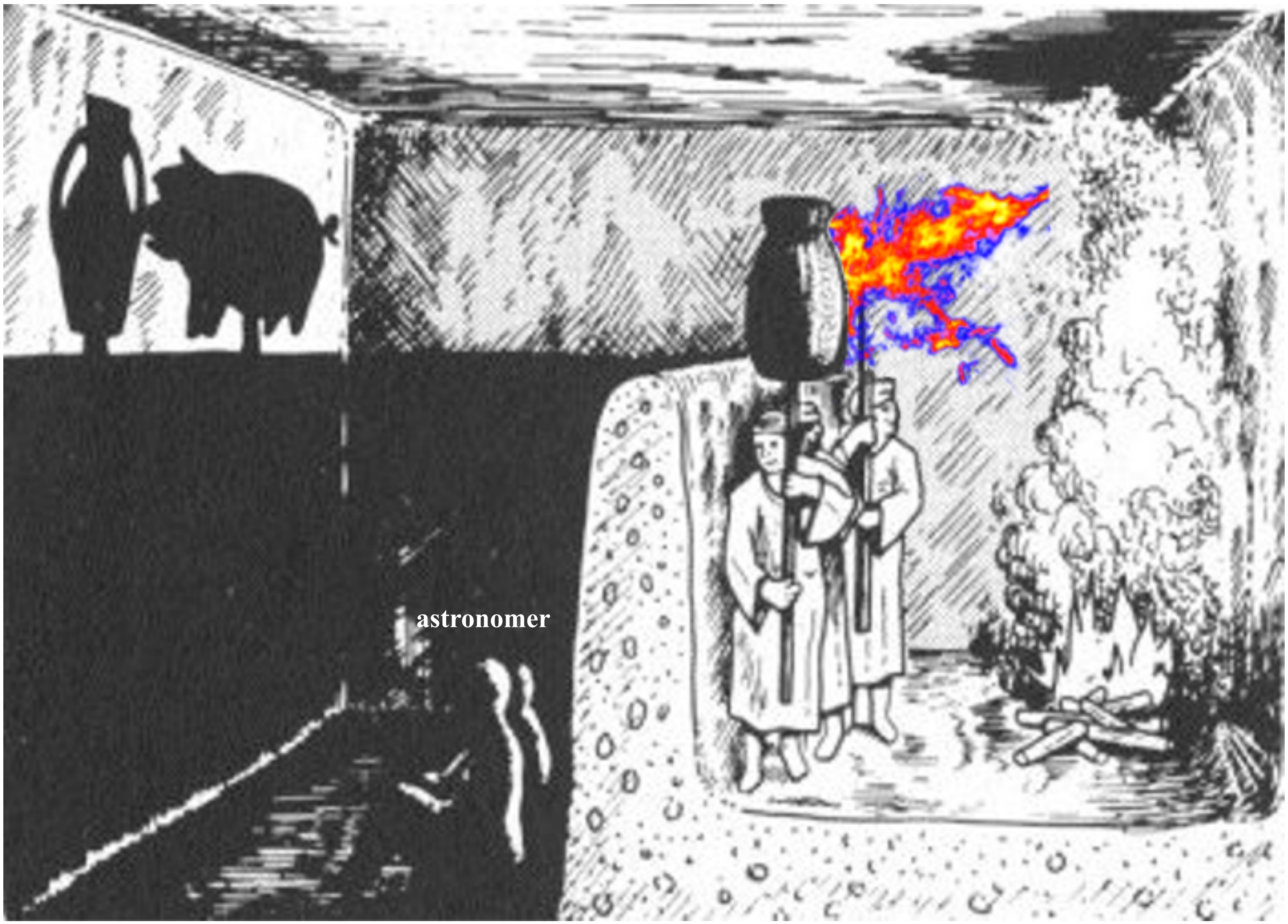

Laszlo Szücs, image from criticalthinking-mc205.wikispaces.com

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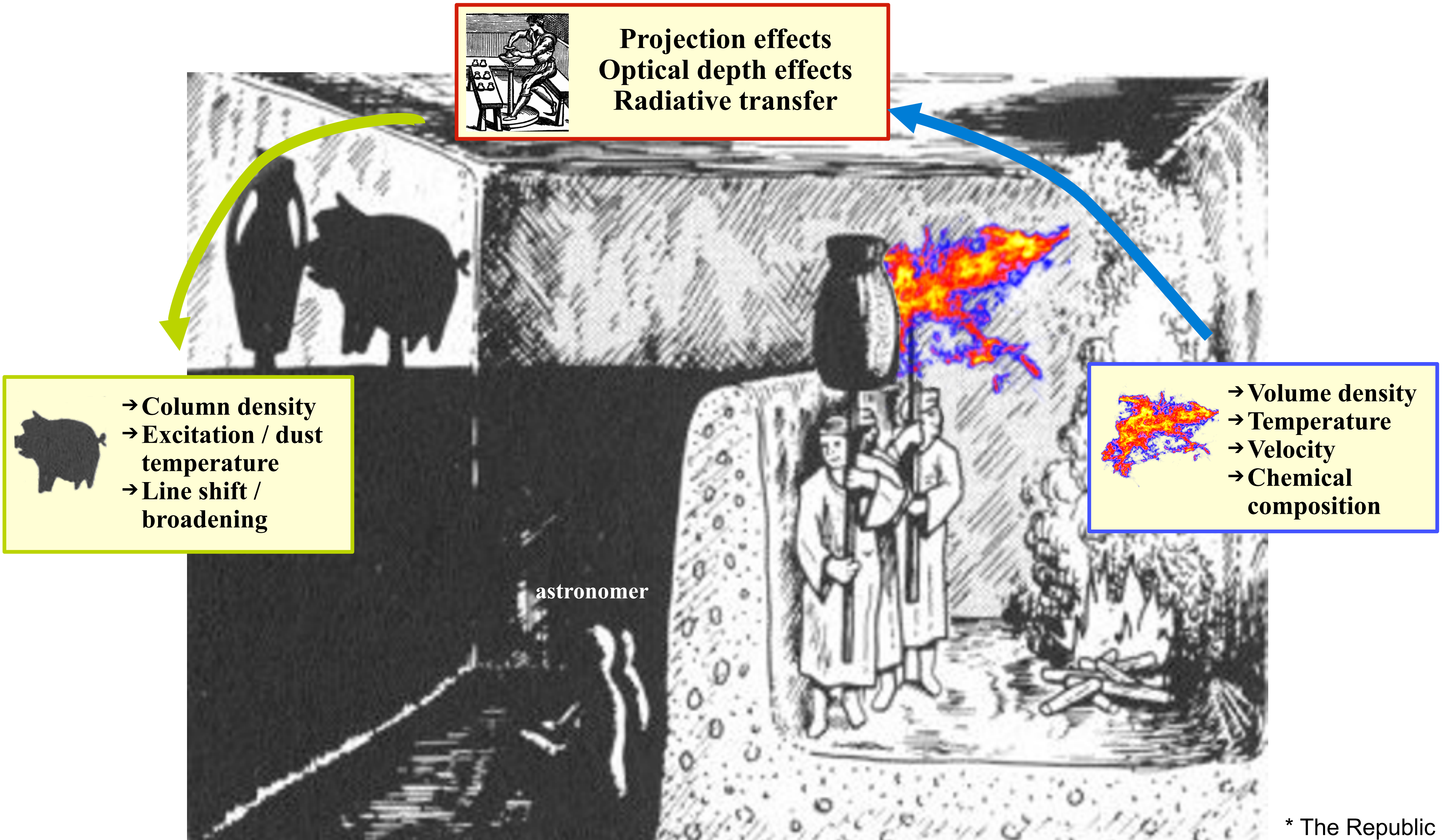

Laszlo Szücs, image from criticalthinking-mc205.wikispaces.com

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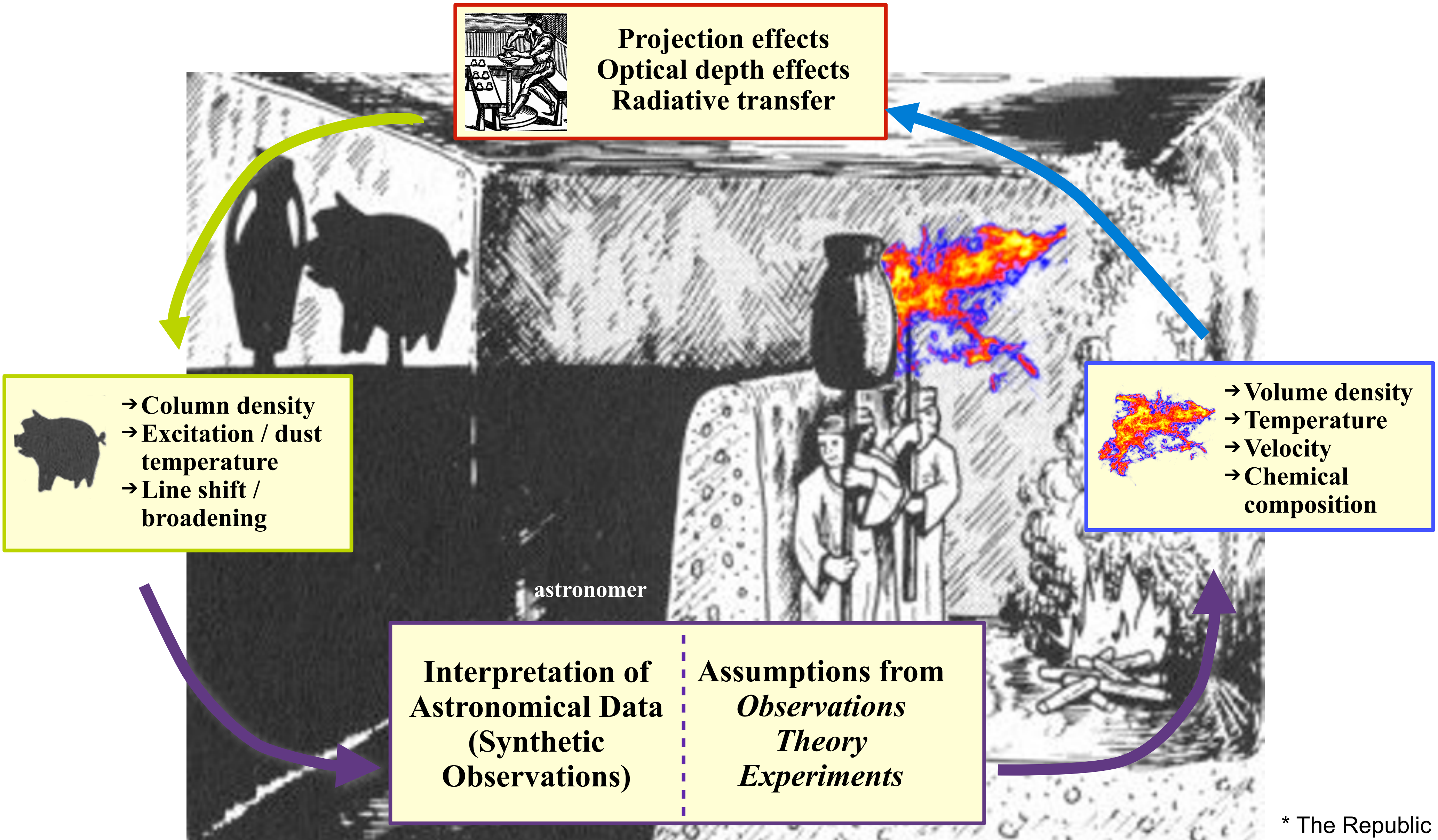
Plato's allegory of the cave* ↔ Astronomical observations

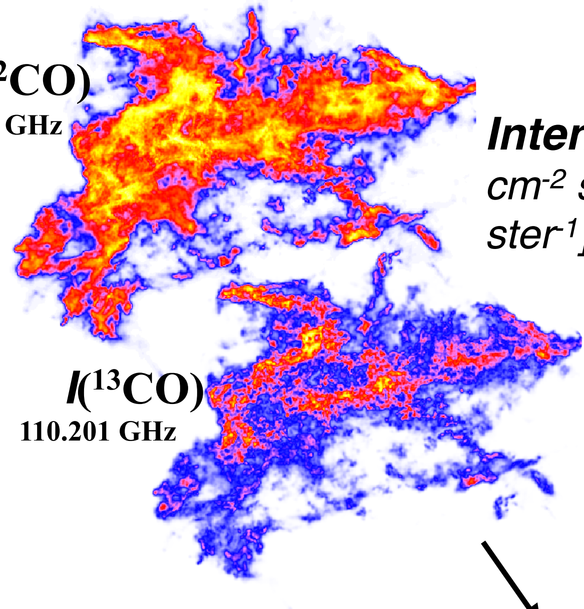


Laszlo Szücs, image from criticalthinking-mc205.wikispaces.com

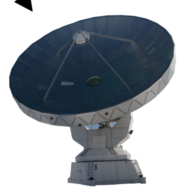
* The Republic (514a-520a)

Example: from CO emission to total column density

J=1-0



Intensity *[erg cm^{-2} s^{-1} Hz^{-1} ster^{-1}]*



Brightness temperature *[K]*

T_B^{12}

T_B^{13}

Following Wilson et al. 2009

Assumptions I.

I(^{12}CO) is optically thick

I(^{13}CO) is optically thin

Along a line of sight uniform T_{ex} and same for ^{12}CO and ^{13}CO

$$T_{\rm ex} = 5.5/\ln\left(1 + \frac{5.5}{T_B^{12} + 0.82}\right)$$

$$\tau_{13}(v) = -\ln\left[1 - \frac{T_{\rm B}^{13}}{5.3}\left\{\exp\left(\frac{5.3}{T_{\rm ex}} - 1\right)^{-1} - 0.16\right\}^{-1}\right]$$

LTE

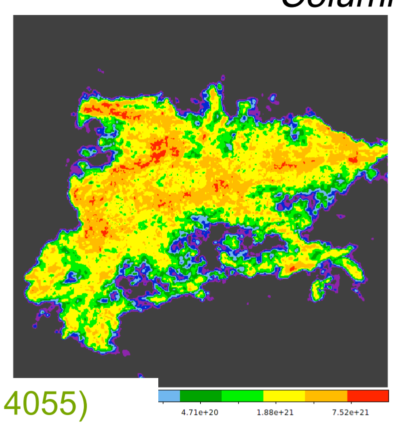
$$N(^{13}{\rm CO}) = 3.0 \times 10^{14} \frac{T_{\rm ex}\int \tau_{13}(v)dv}{1 - \exp(-5.3/T_{\rm ex})}$$

Assumptions II.

Uniform N(^{12}CO)/N(^{13}CO) ~ 60 *

N(H_2)/N(^{12}CO) ratio ~ 6.6×10^3 **

Column density [cm^{-2}]

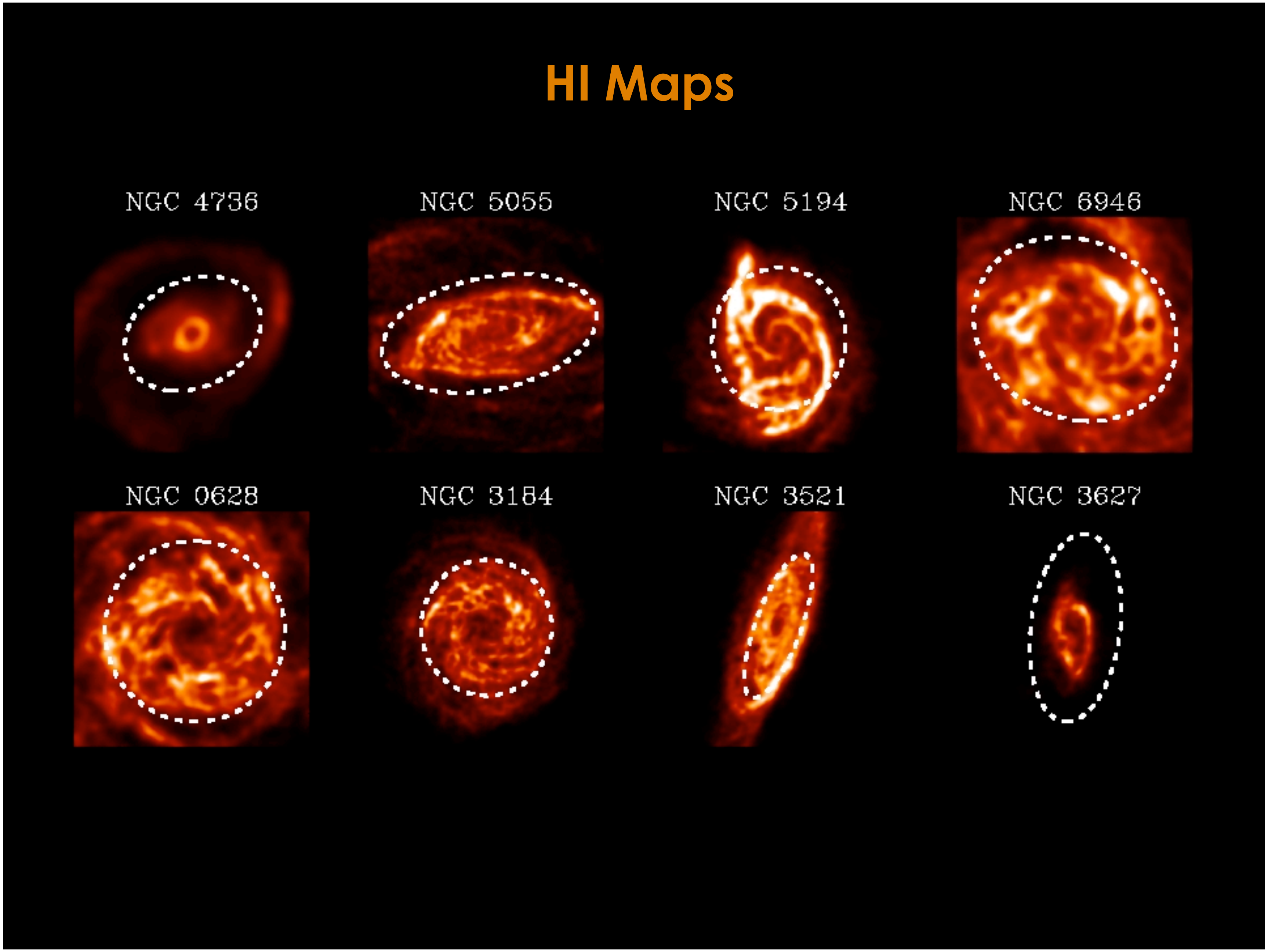


Astrophysical interpretation

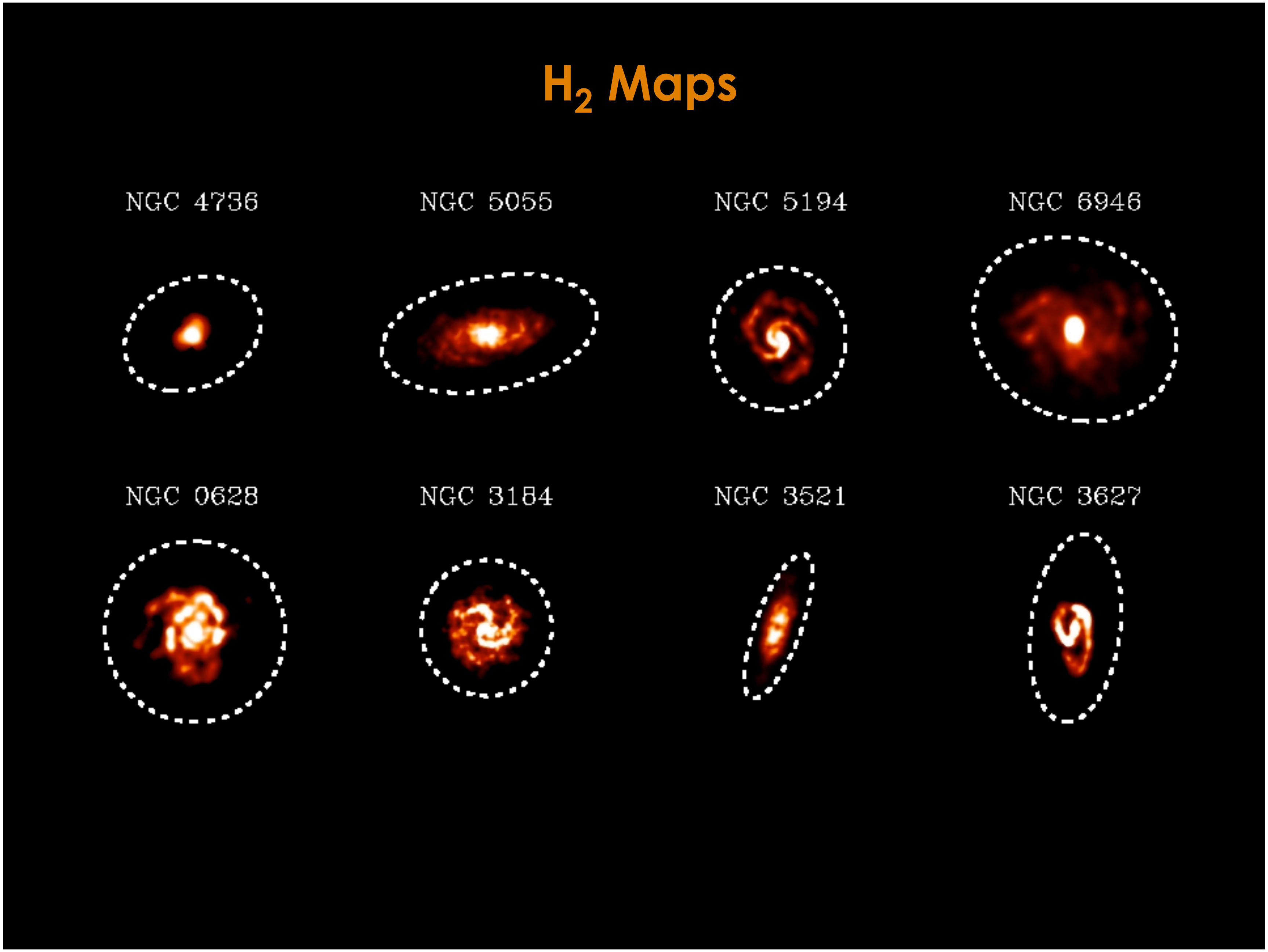
Laszlo Szücs et al. (2014, MNRAS, 445, 4055)

* Langer & Penzias (1990)
** Pineda et al. (2009)

global SF relations



galaxies from THINGS and HERACLES survey
(images from Frank Bigiel, ZAH/ITA)



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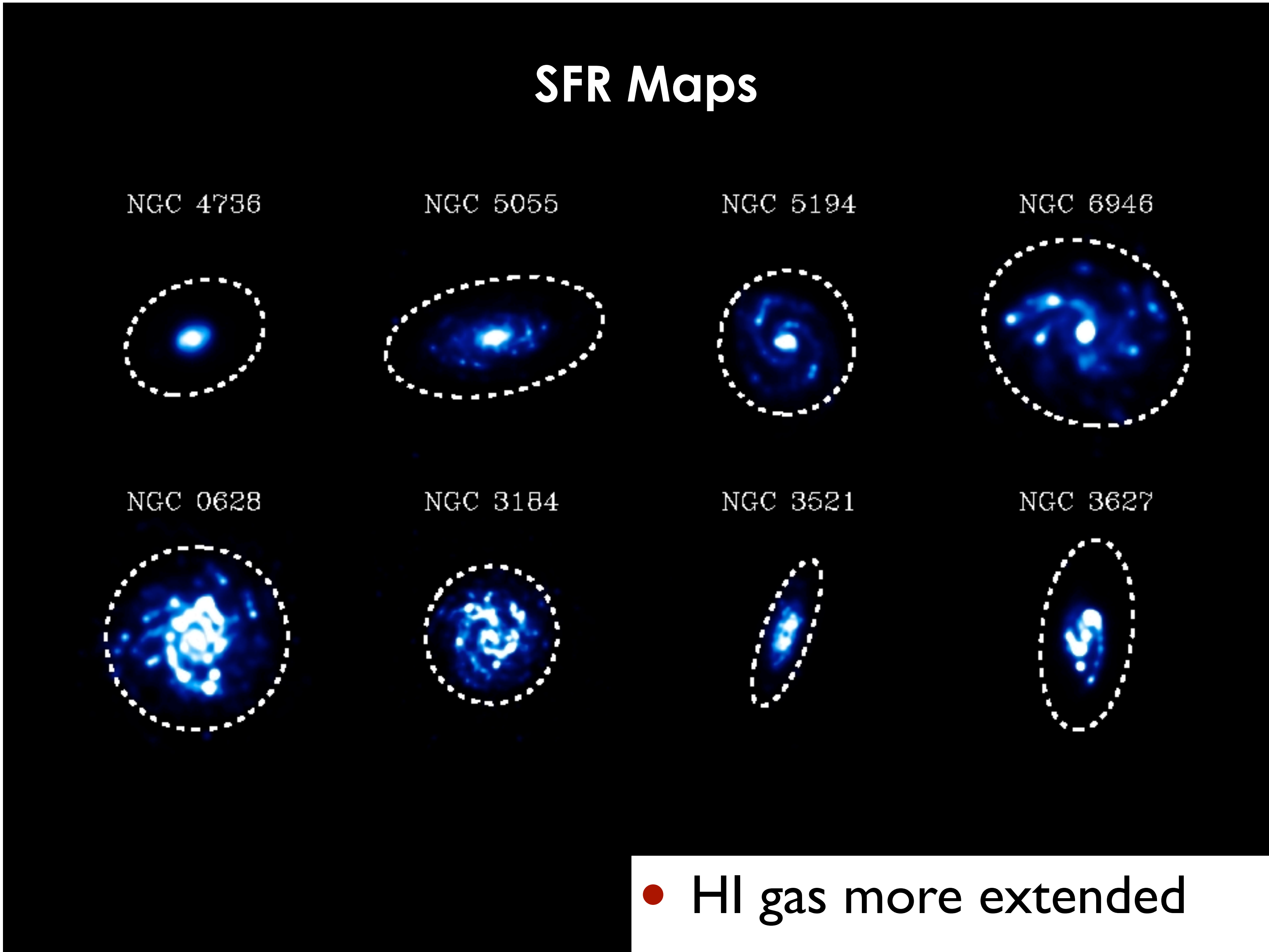
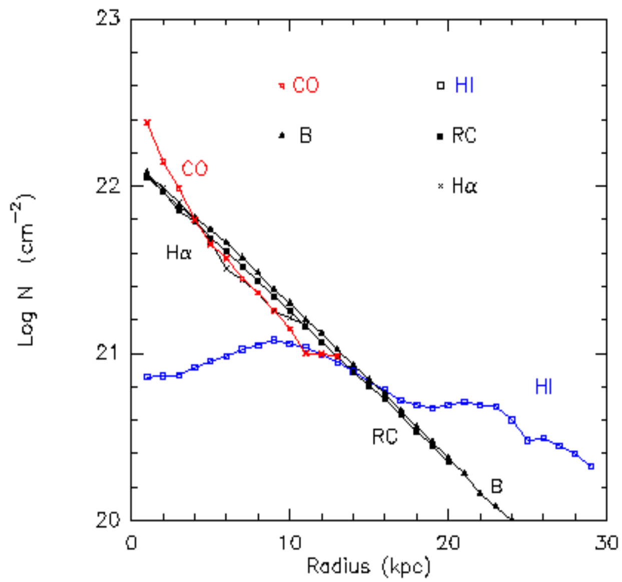


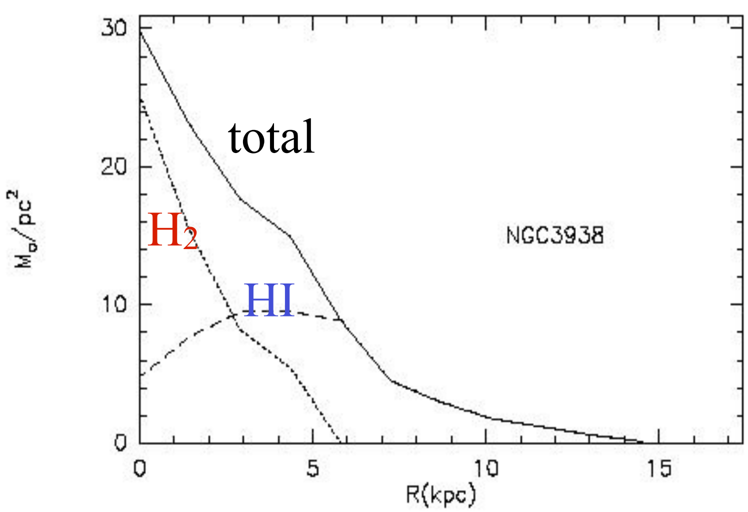
- HI gas more extended
- H2 and SF well correlated

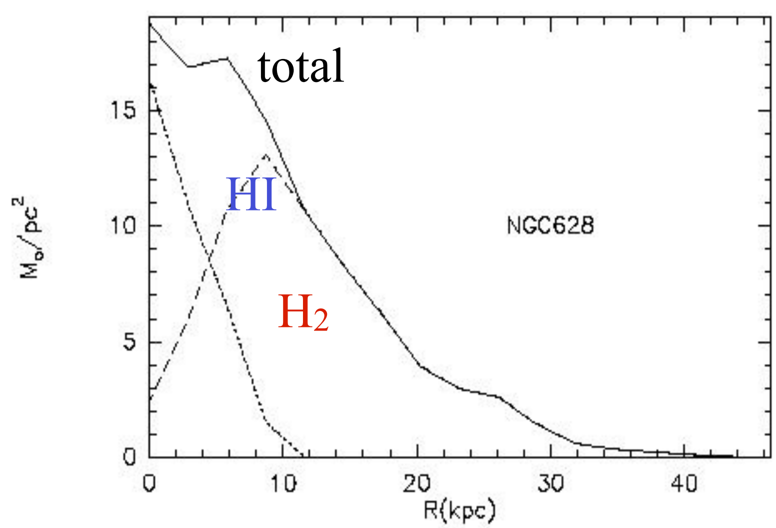
galaxies from THINGS and HERACLES survey
(images from Frank Bigiel, ZAH/ITA)

1. radial distribution in spirals

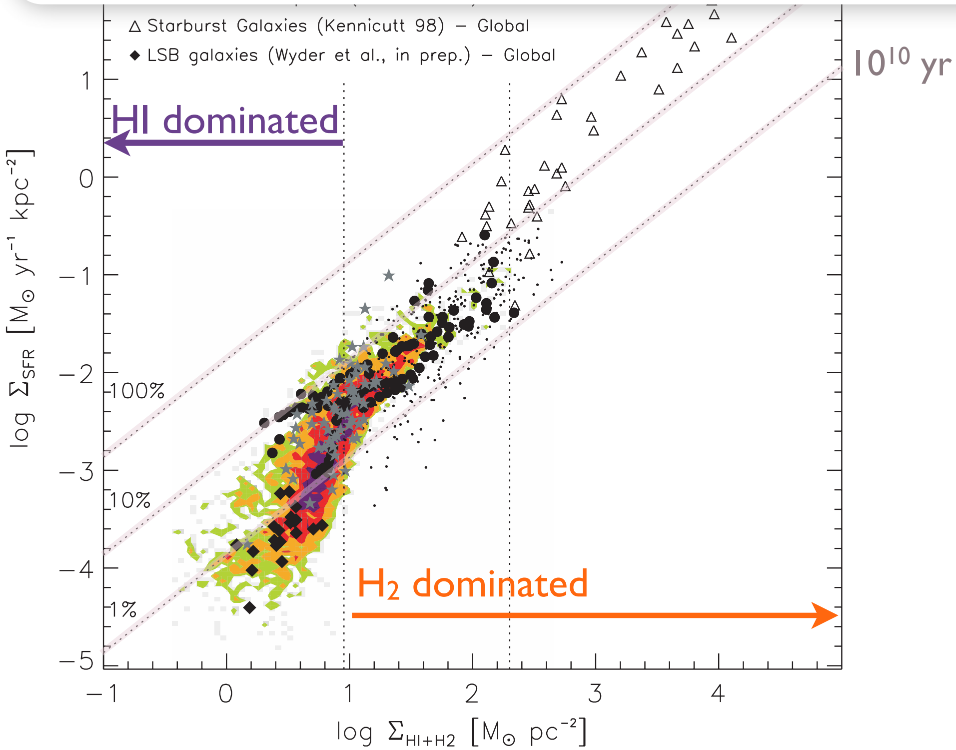
- HI versus H_2:
  - H_2 is restricted to the optical disk
  - while the HI extends 2 - 4 x optical radius
- HI hole or depression in the centers, sometimes compensated by H_2
- often H_2 is exponential like stars, HI does *not* follow in most cases



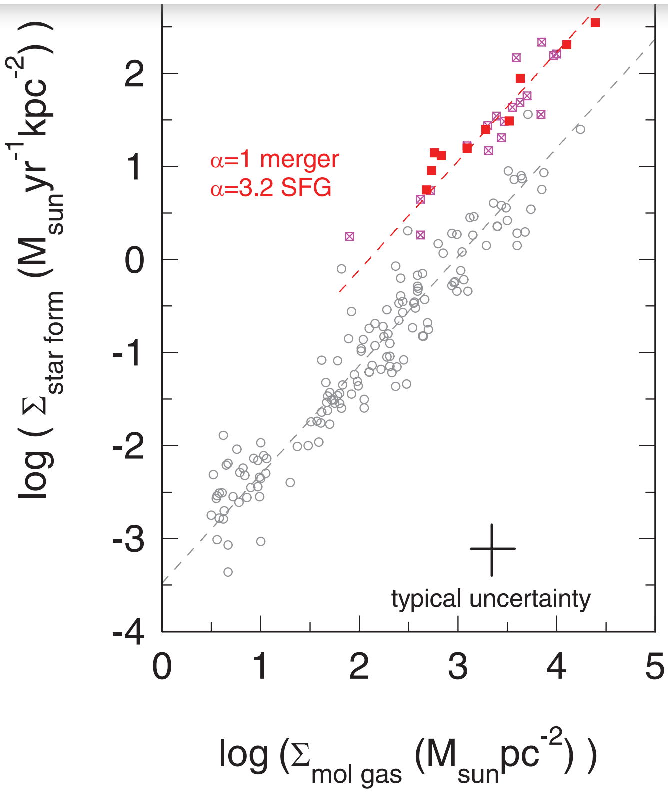




2. correlation with star formation



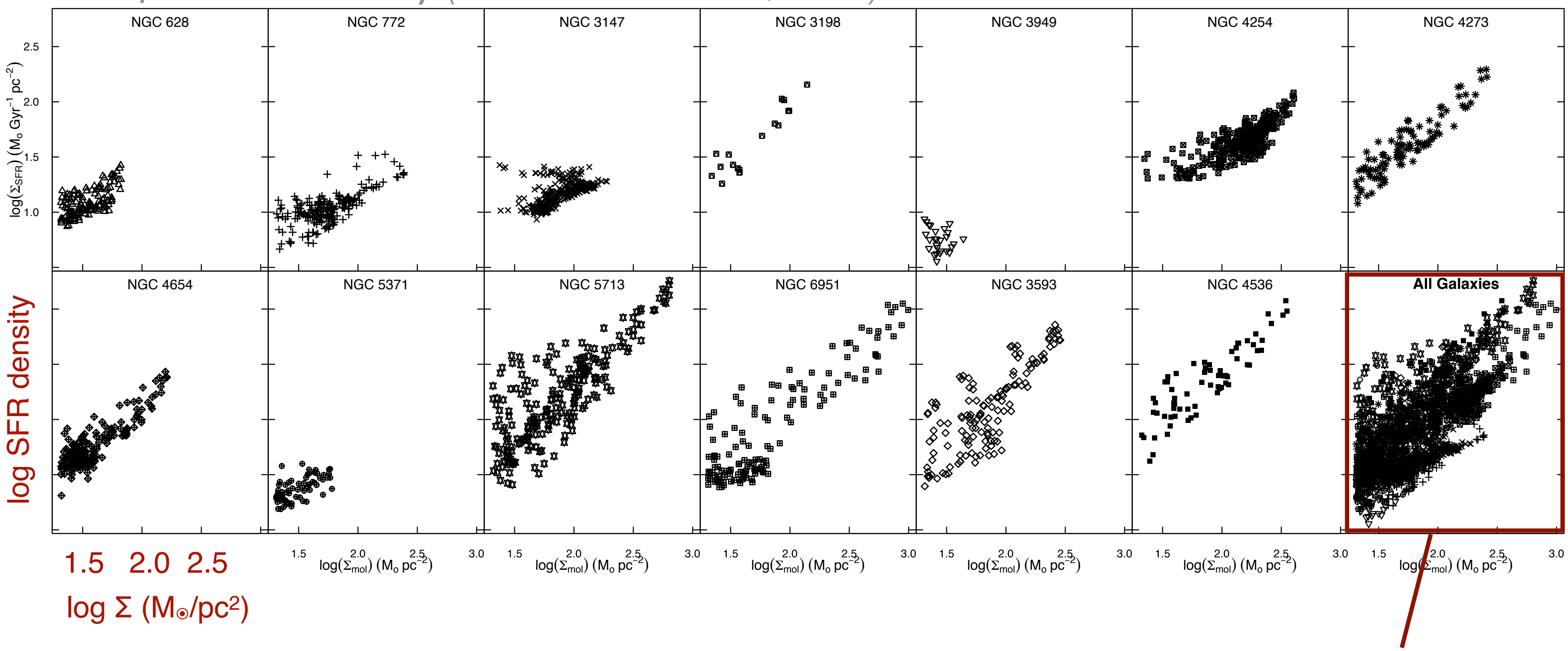
Bigiel et al. (2008, AJ, 136, 2846)



Genzel et al. (2010, MNRAS, AJ, 407, 2091)

- standard model: roughly linear relation between H
- standard model: roughly constant depletion time: few x 10
- super linear relation between total gas and SFR

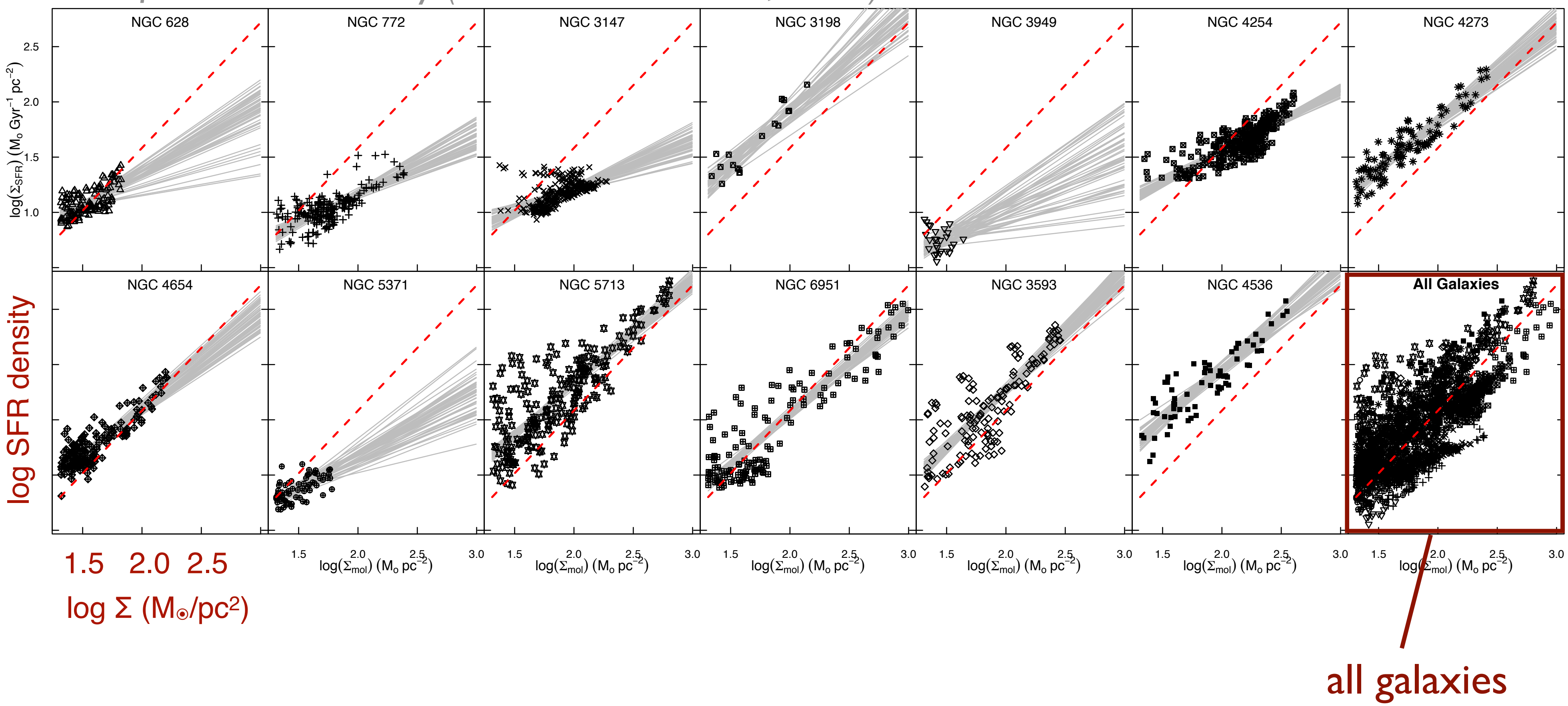
data from STING survey (Rahman et al. 2011, 2012)



- QUIZ: do you see a universal

Shetty et al. (2014, MNRAS, 437, L61, see also Shetty, Kelly, Bigiel, 2013, MNRAS, 430, 288)

data from STING survey (Rahman et al. 2011, 2012)



- QUIZ: do you see a universal
- ANSWER: - probably not
  - in addition, the relation often is sublinear

Shetty et al. (2014, MNRAS, 437, L61, see also Shetty, Kelly, Bigiel, 2013, MNRAS, 430, 288)

Hierarchical Bayesian models give more reliable estimates of the *slope* and the *intercept* of a power-law fit compared to least-square fits (or bisector fits).

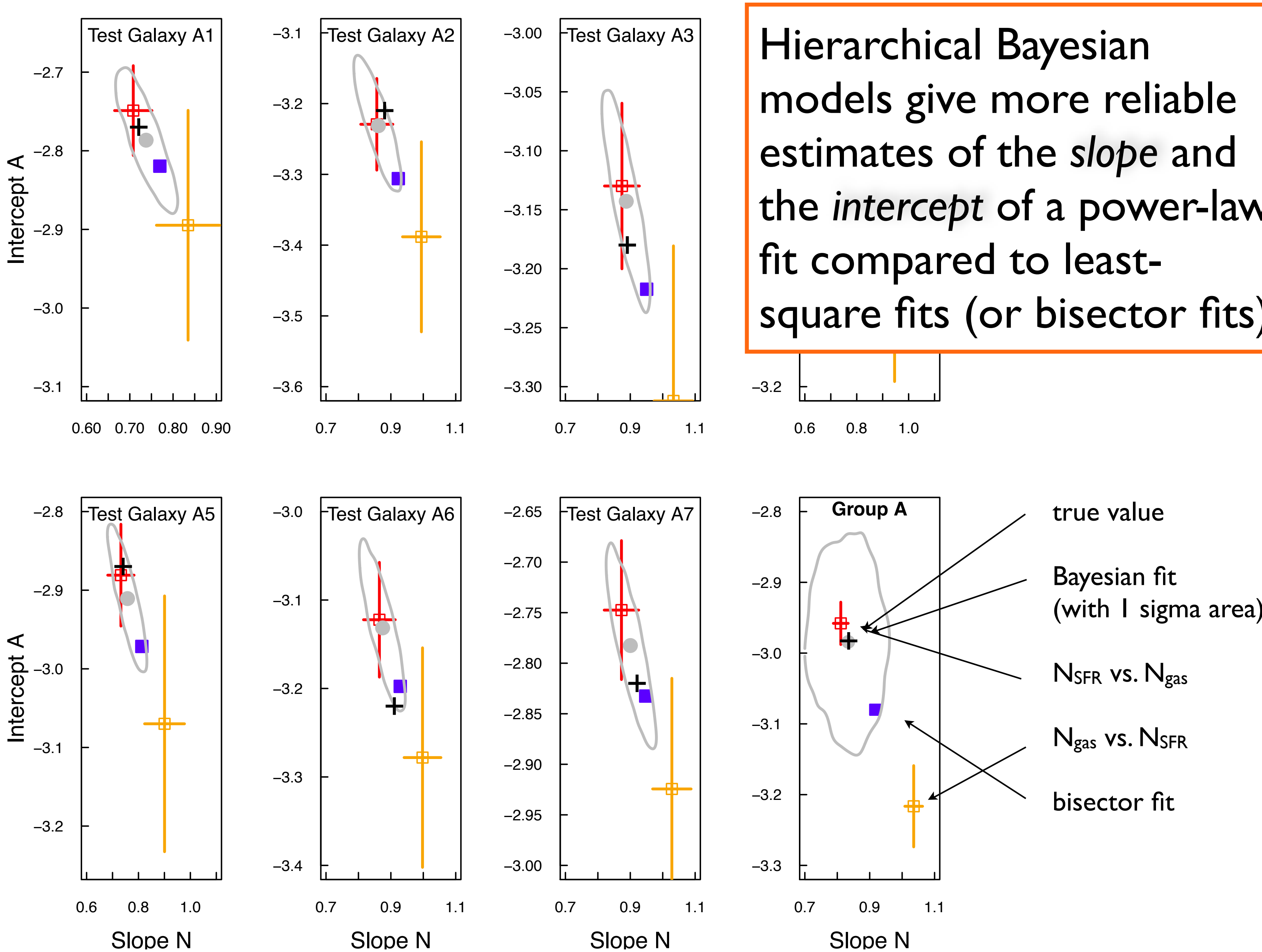
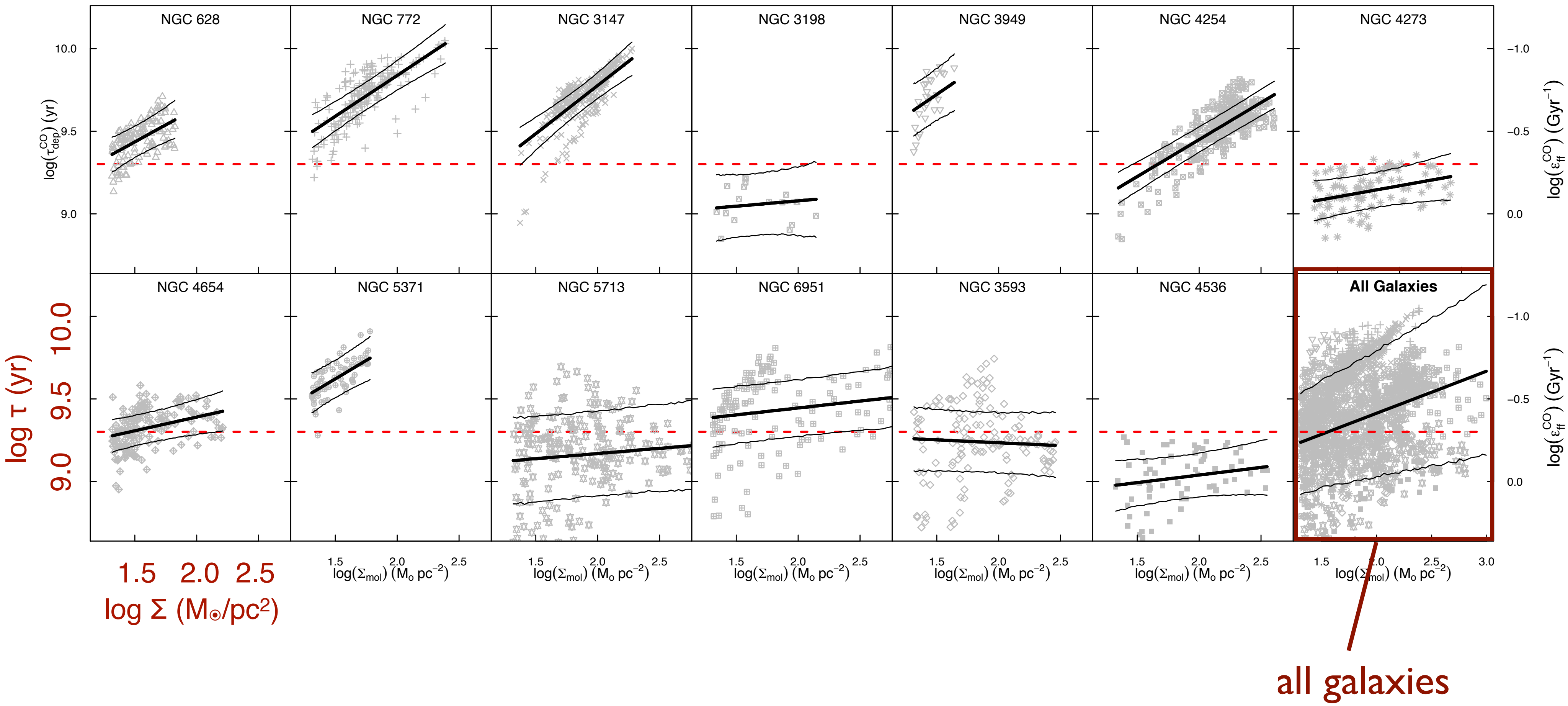


Figure 1. Slope and intercept of test galaxies in Group A. Black cross shows the true values. Red and orange squares show the OLS($\Sigma_{\rm SFR}|\Sigma_{\rm mol}$) and OLS($\Sigma_{\rm mol}|\Sigma_{\rm SFR}$) results, with their 1σ uncertainties, respectively. The gray circles indicate the estimate provided by the median of hierarchical Bayesian posterior result, and the contours mark the 1σ deviation. The filled blue squares mark the bisector estimates. The last panel on the bottom row shows the group parameters and fit estimates.

Shetty et al. (2013, MNRAS, 430, 288)

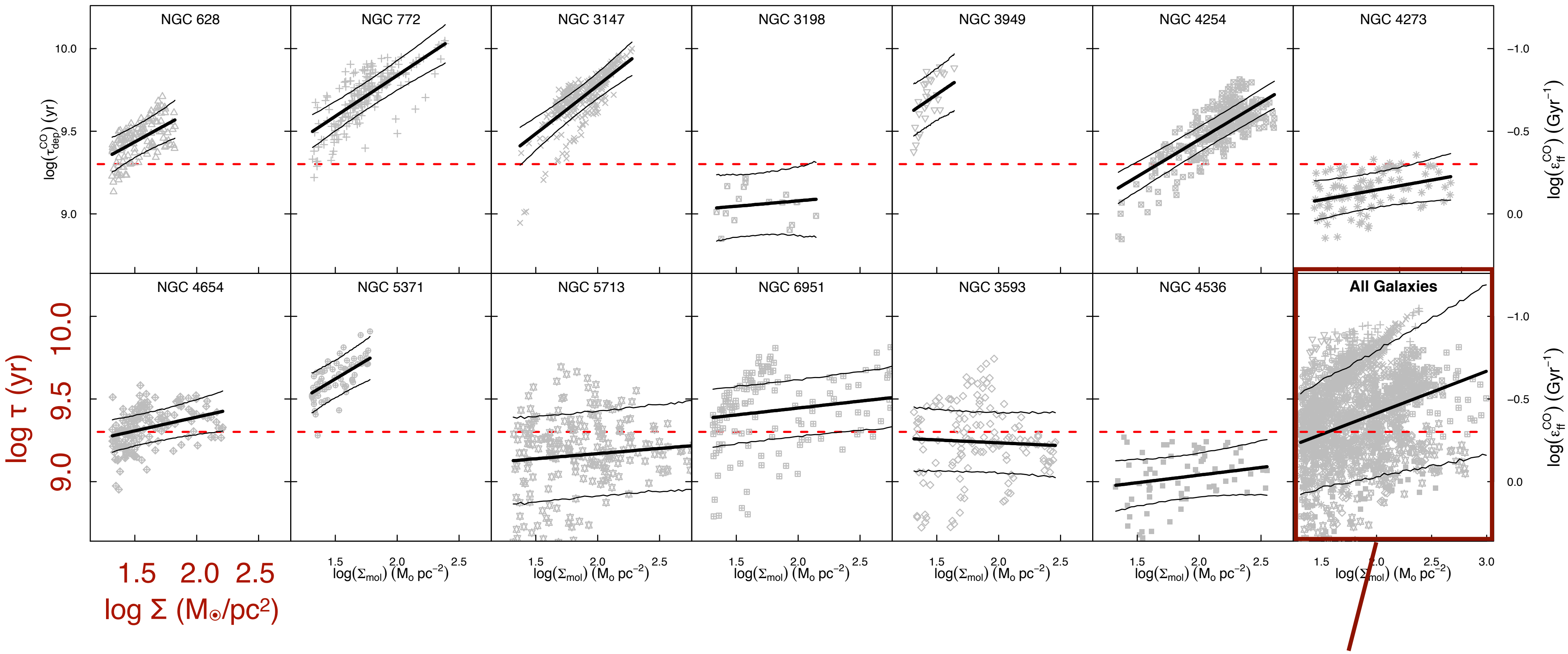
data from STING survey (Rahman et al. 2011, 2012)



Hierarchical Bayesian model for STING galaxies indicate *varying depleting times*.

Shetty et al. (2014, MNRAS, 437, L61)

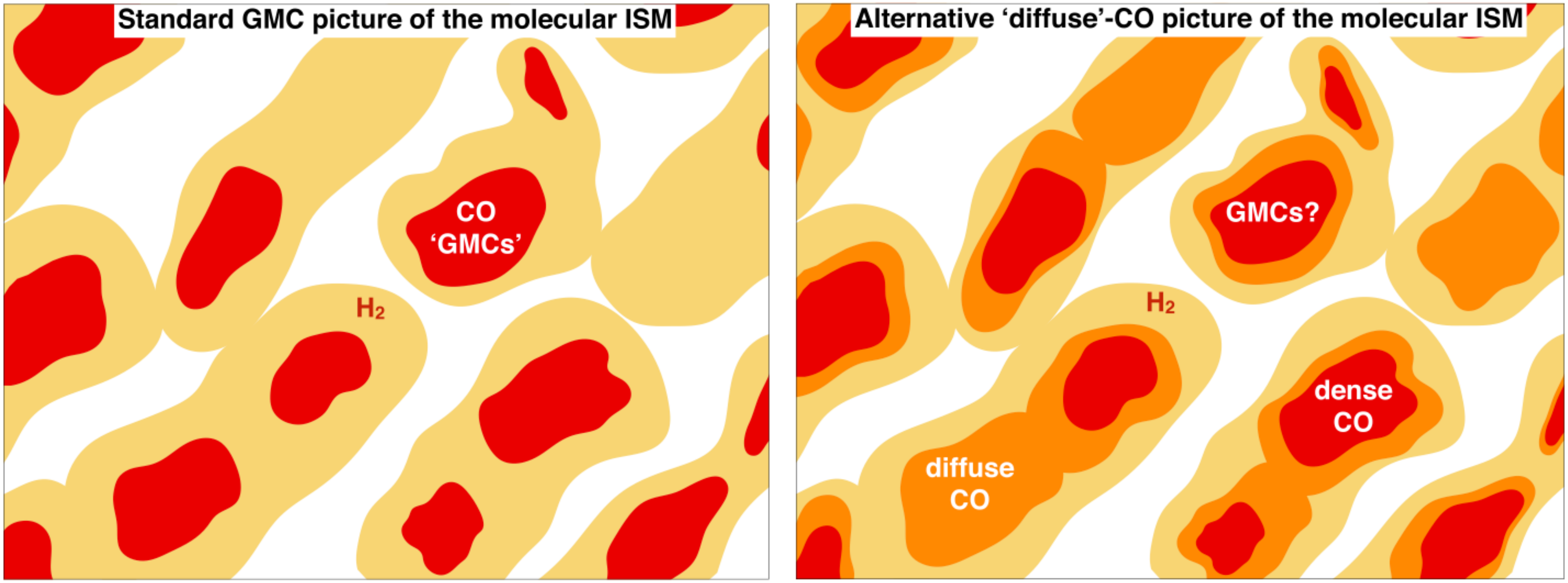
data from STING survey (Rahman et al. 2011, 2012)



physical origin of this behavior?

- maybe strong shear in dense arms (example M51, Meidt et al. 2013)...
- maybe non-star forming H
  densities (recall H

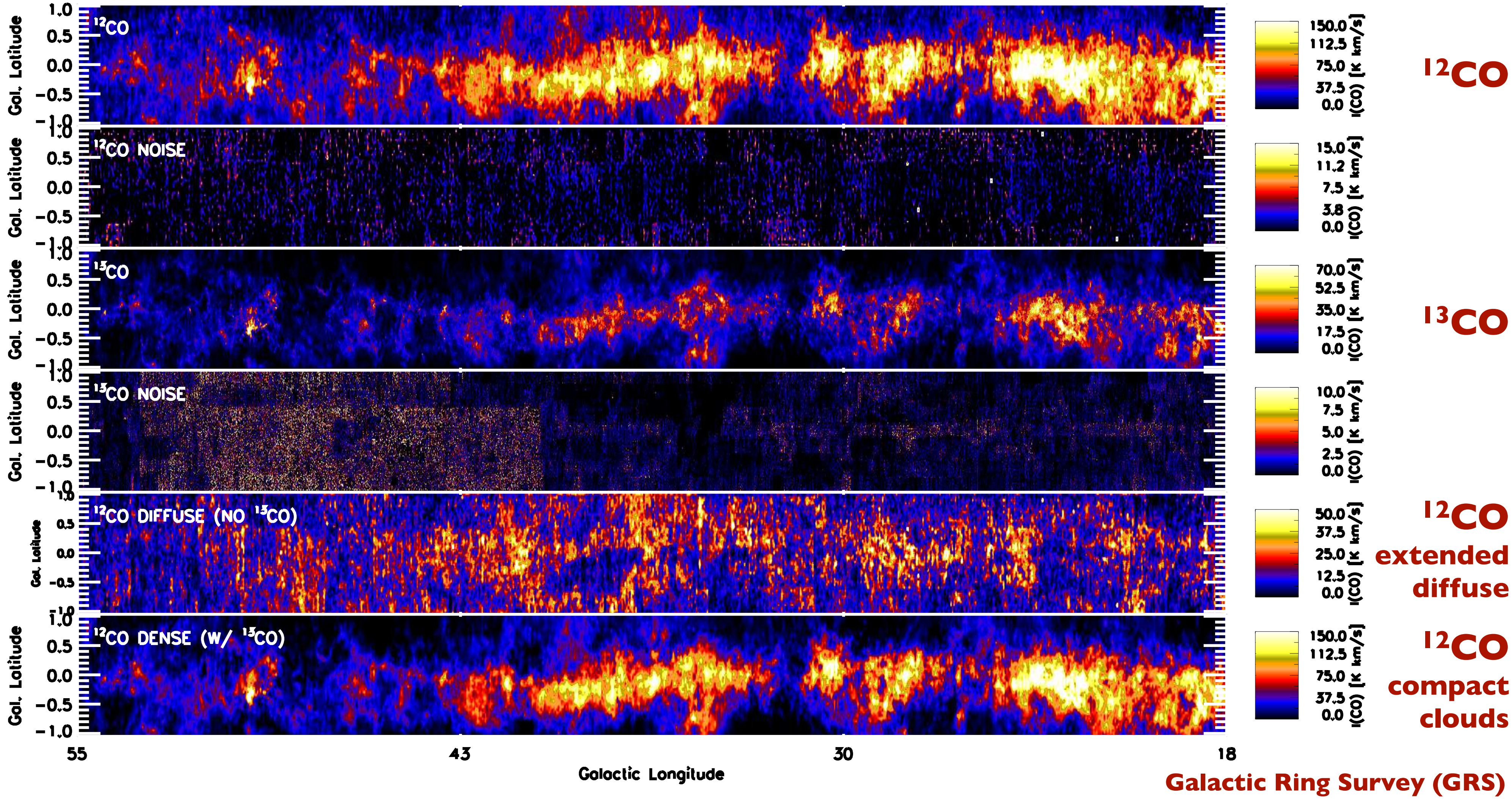
Shetty et al. (2013, MNRAS, 437, L61, see also Shetty, Kelly, Bigiel, 2013, MNRAS, 430, 288)



in addition:

- maybe a large fraction of H
  dense clouds, but in a diffuse state!

Shetty et al. (2014, MNRAS, 422, 2208)



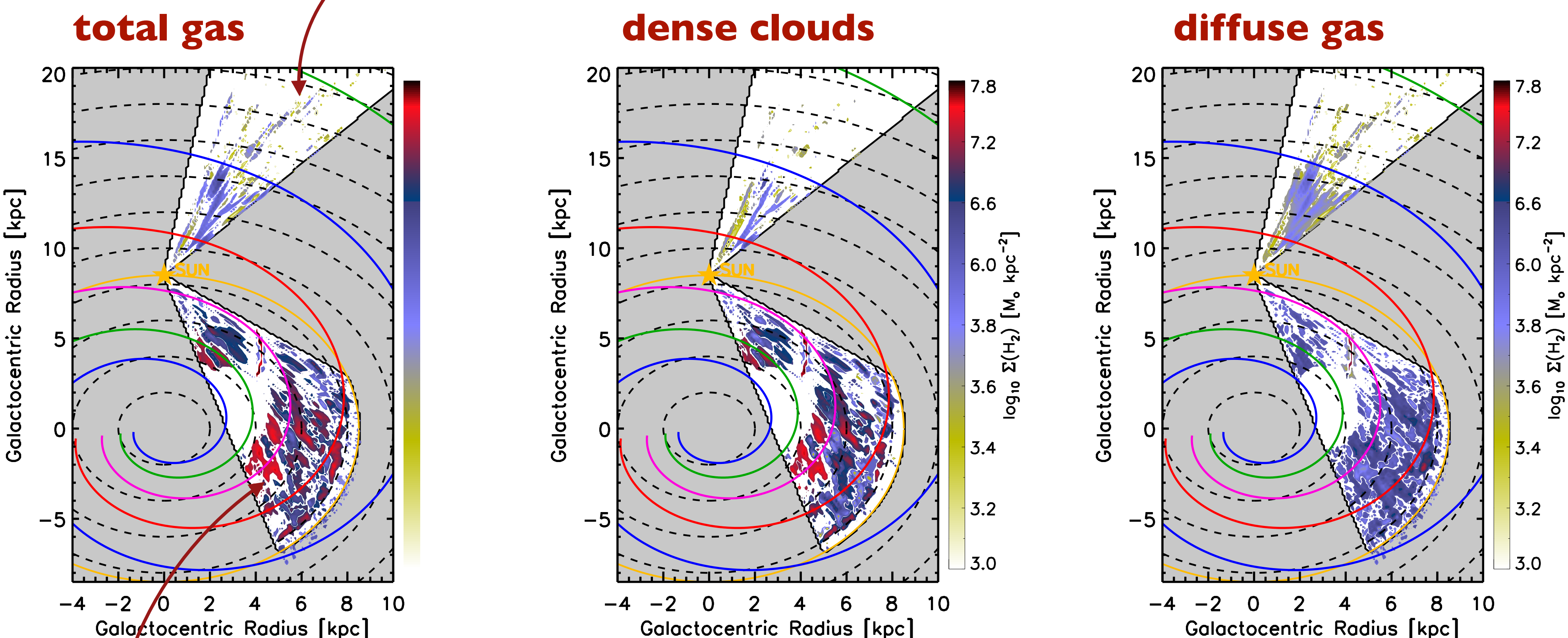
in addition:

- comparison of
  tracing all the gas (including the more diffuse component)

Roman-Duval et al. (2015, in prep.)

Spacial distribution

OUTER GALAXY:
Mark Heyer's survey



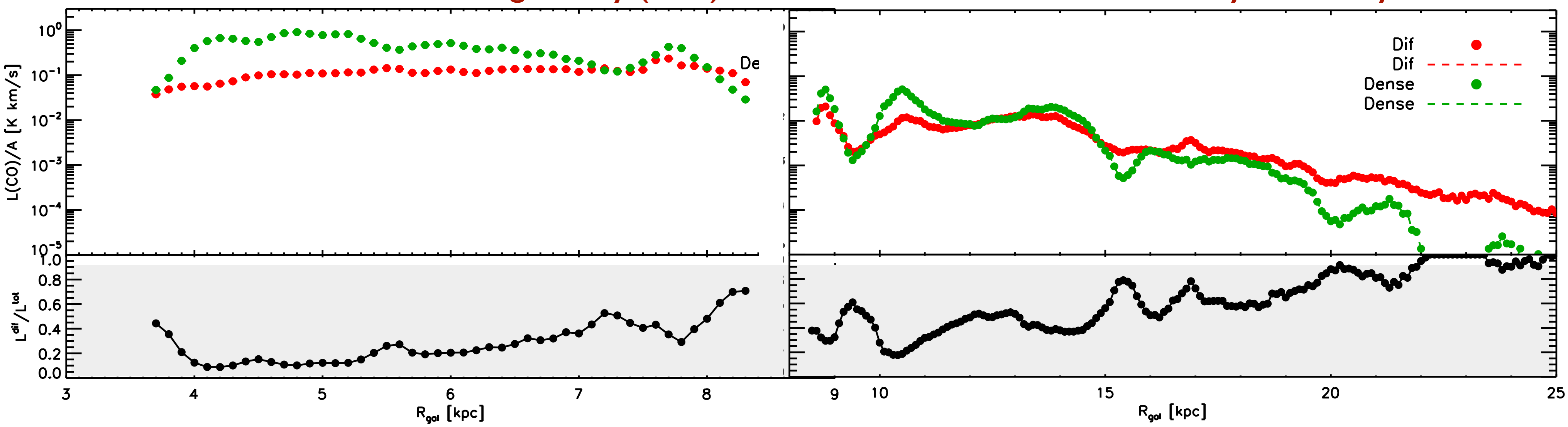
INNER GALAXY:
Galactic Ring Survey (GRS)

Roman-Duval et al. (2015, in prep.)

Diffuse gas fraction as function of Galactic radius.

INNER GALAXY: Galactic Ring Survey (GRS)

OUTER GALAXY: Mark Heyer's survey



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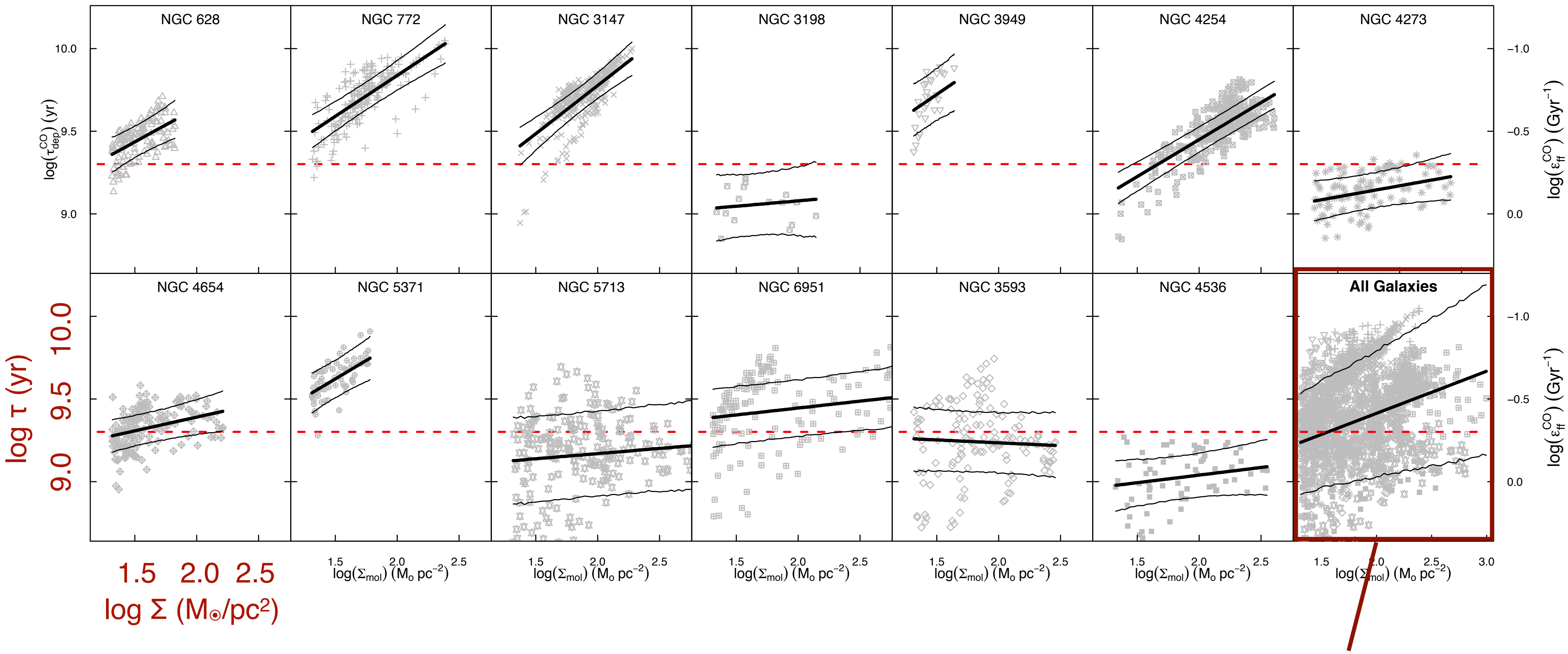

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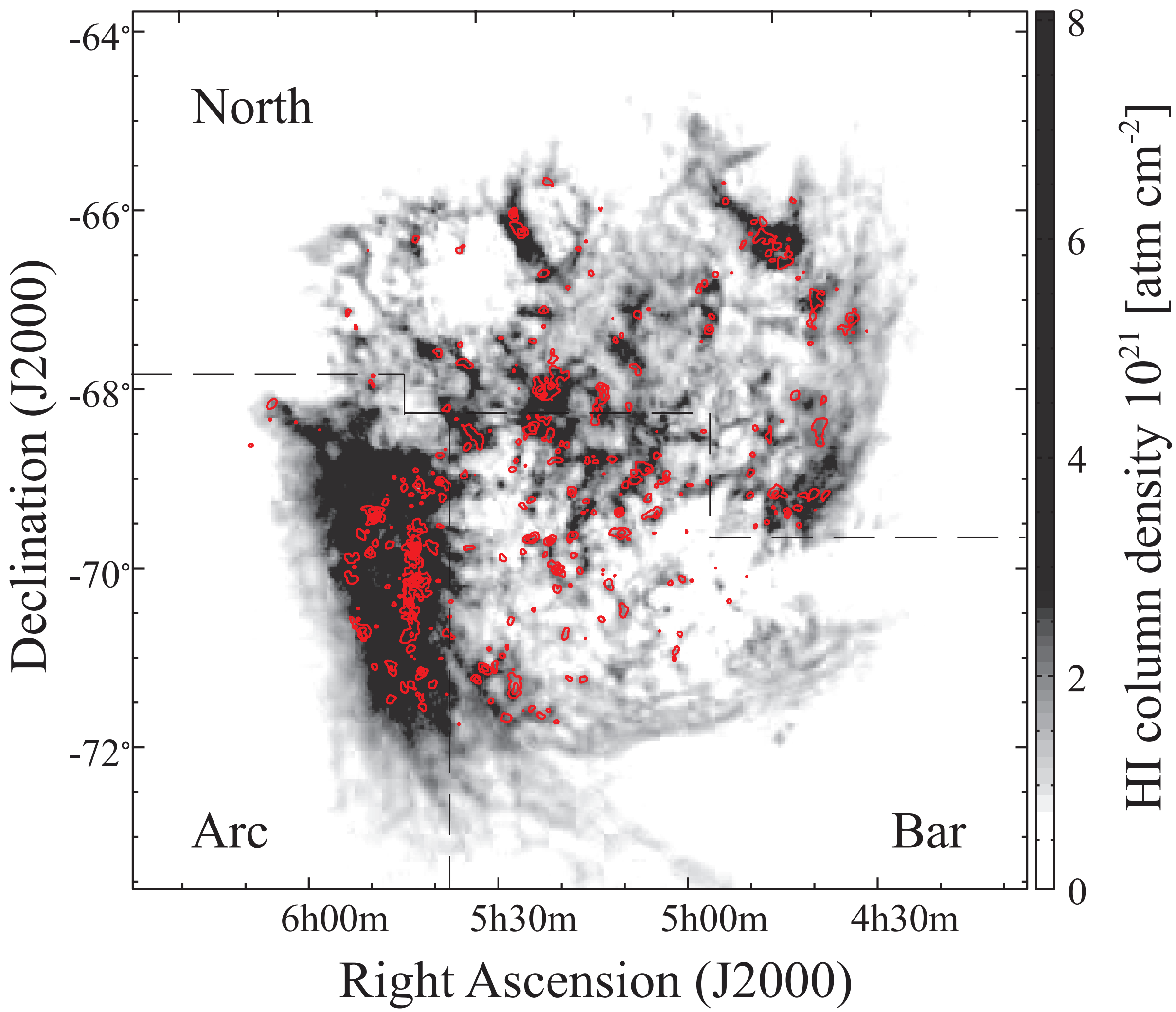
Shetty et al. (2013, MNRAS, 437, L61, see also Shetty, Kelly, Bigiel, 2013, MNRAS, 430, 288)

molecular cloud formation

molecular cloud formation



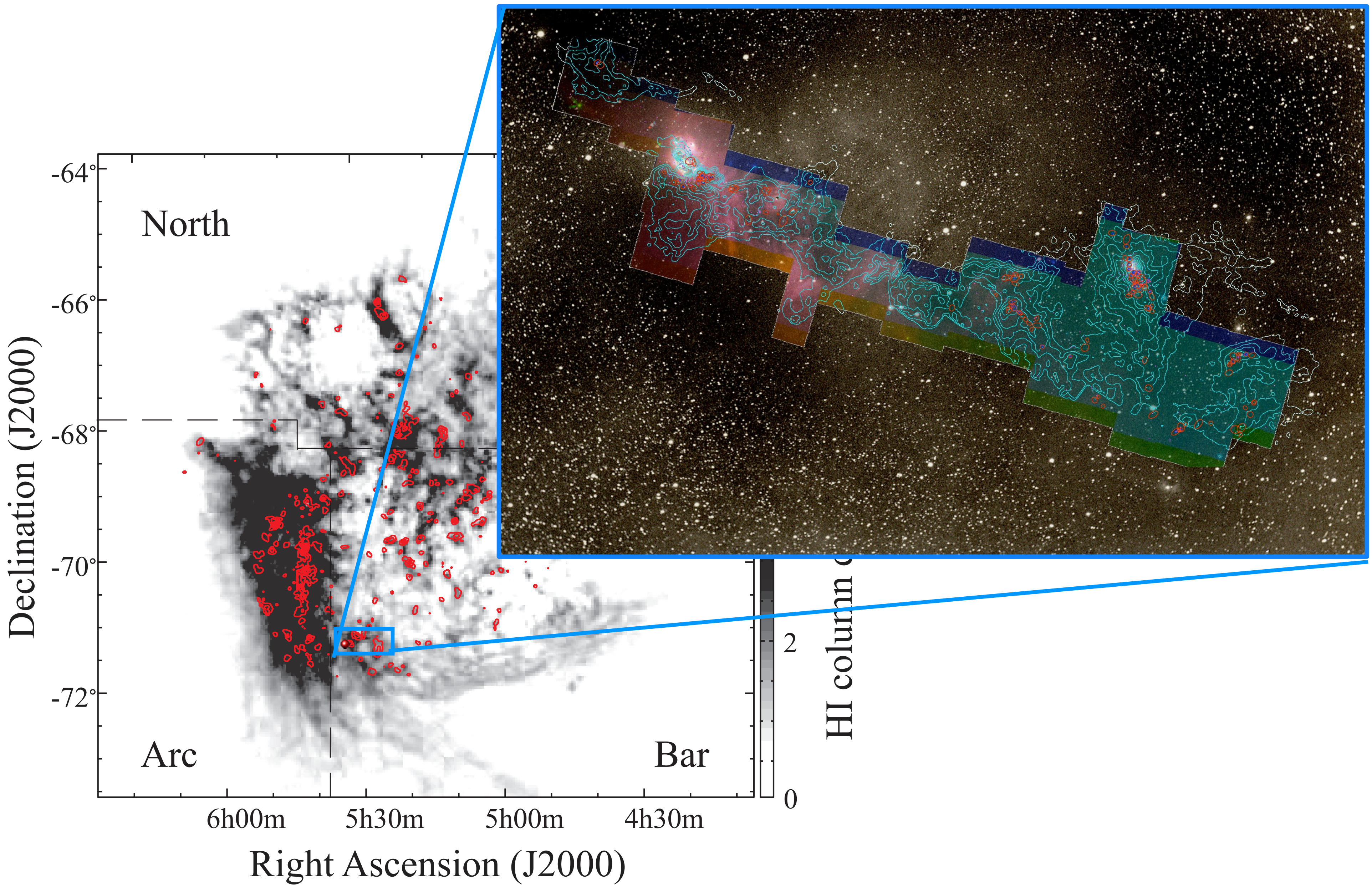
Idea:

Molecular clouds form at *stagnation points* of large-scale convergent flows, mostly triggered by global (or external) perturbations. Their internal turbulence is driven by accretion, i.e. by the process of cloud formation

- molecular clouds grow in mass
- this is inferred by looking at molecular clouds in different evolutionary phases in the LMC (Fukui et al. 2008, 2009)

Fukui et al. (2009)

zooming in ...


-64°
-66°
-68°
-70°
-72°
North
Arc
Bar
Declination (J2000)
6h00m
5h30m
5h00m
4h30m
Right Ascension (J2000)
2
0
HI column

position-position-velocity structure of the Perseus cloud

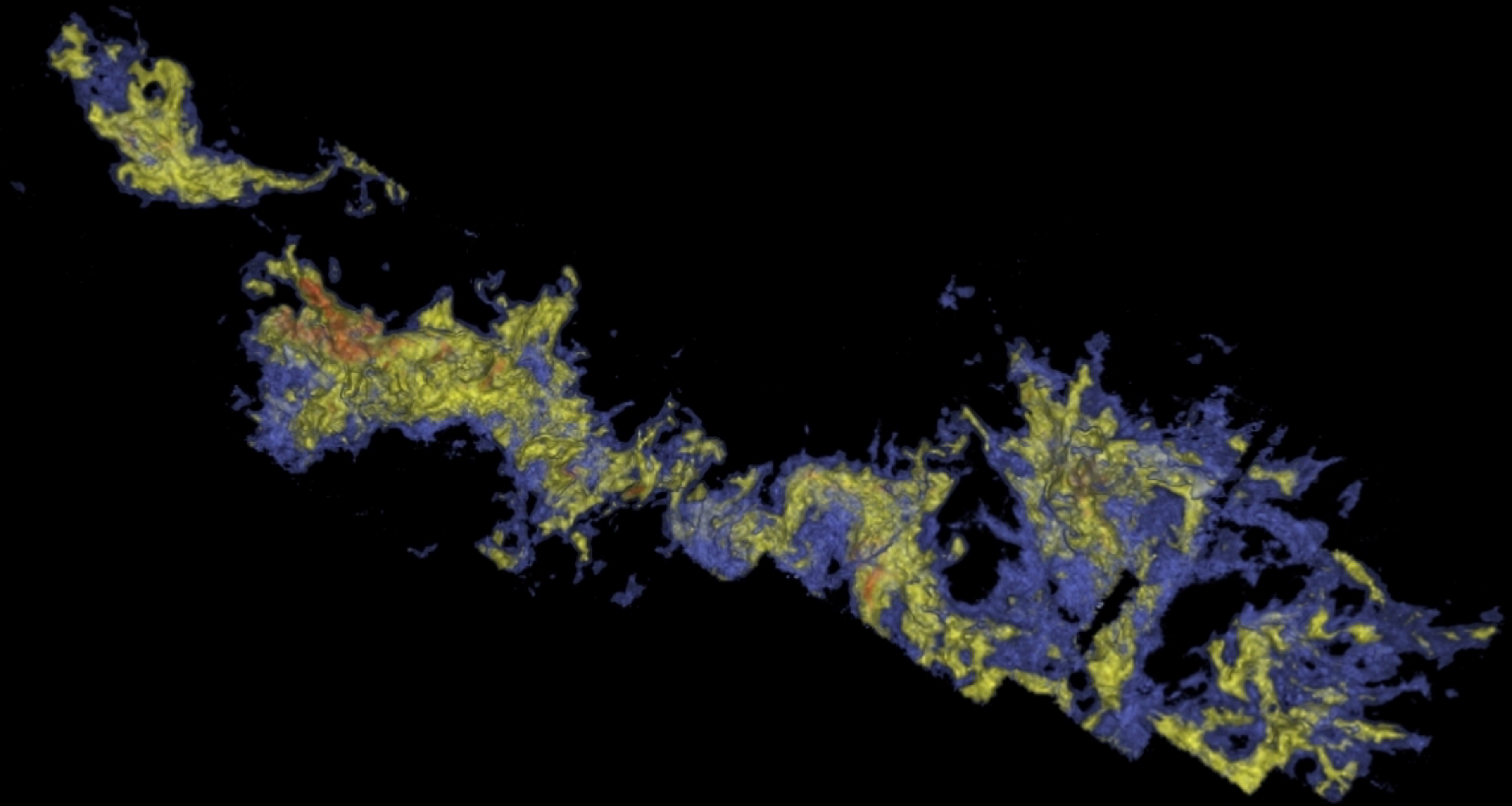
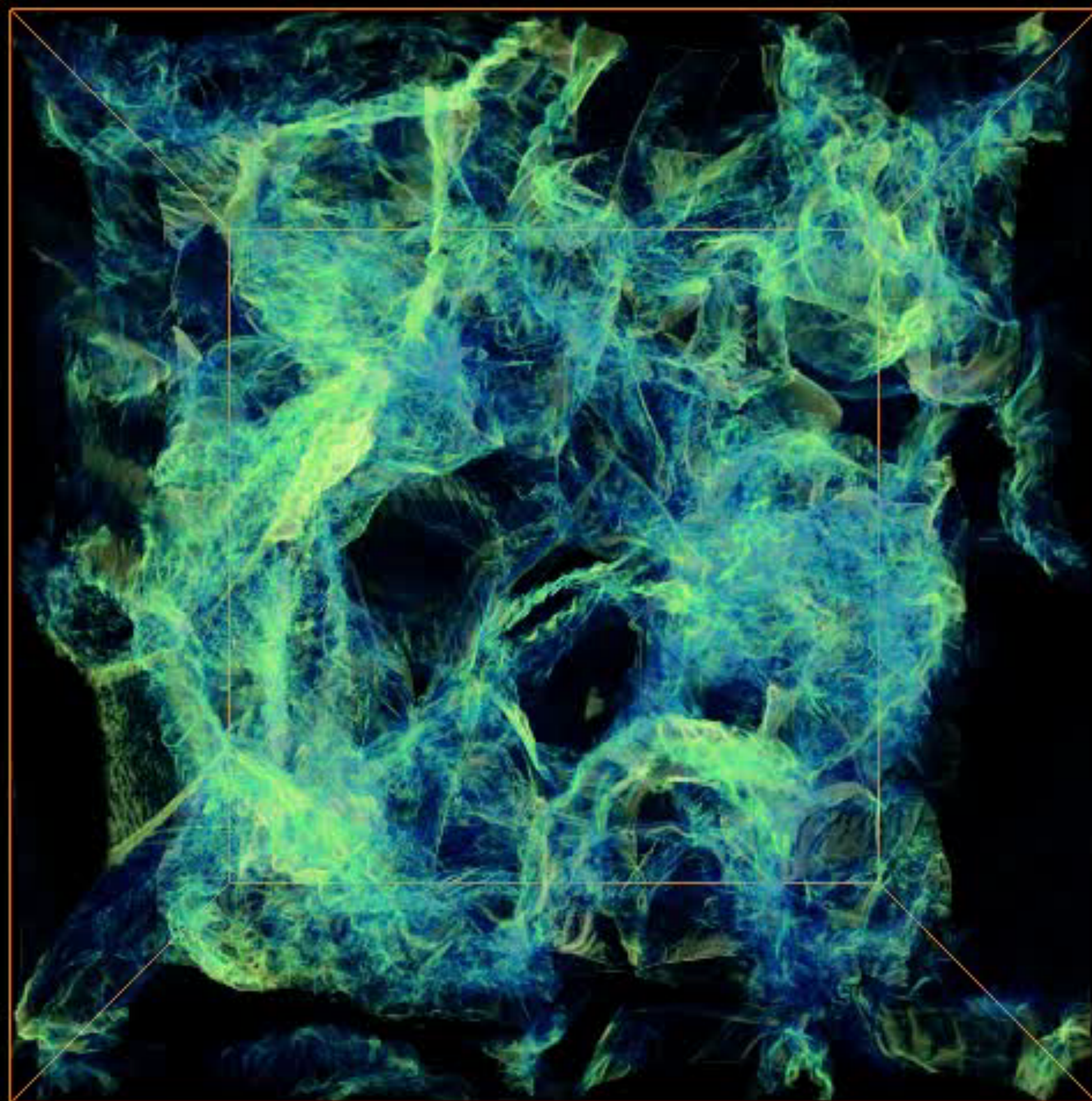


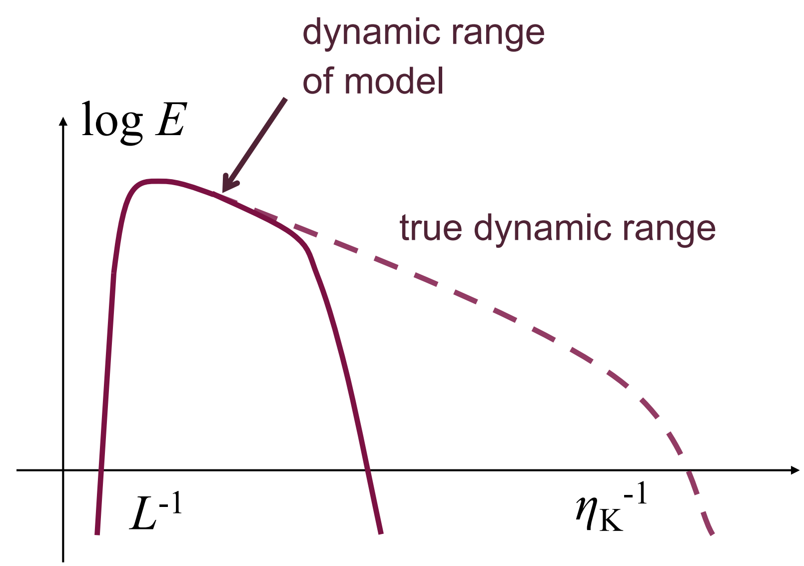
image from Alyssa Goodman: COMPLETE survey



Schmidt et al. (2009, A&A, 494, 127)

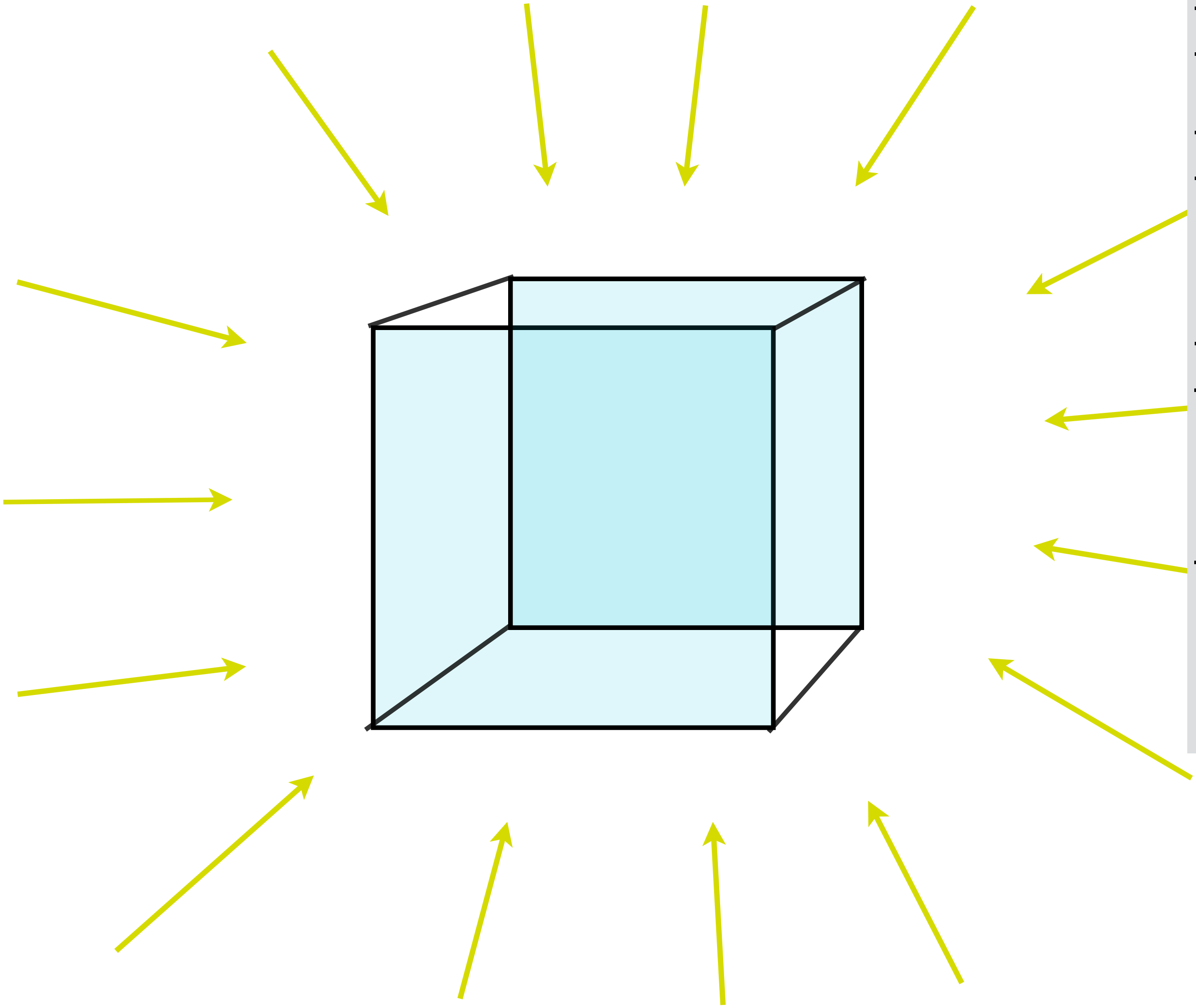
caveat of numerical simulations

- most astrophysical turbulence simulations use an ***LES*** approach to model the flow
- principal problem: only large scale flow properties
  - Reynolds number: Re = LV/ν ***(Re_{nature} >> Re_{model})***
  - dynamic range much smaller than true physical one
  - need *subgrid model* (often only dissipation)
  - but what to do for more complex when processes on subgrid scale determine large-scale dynamics (chemical reactions, nuclear burning, etc)
  - Turbulence is "space filling" --> difficulty for AMR (don't know what criterion to use for refinement)
- how *large* a Reynolds number do we need to catch basic dynamics right?



including detailed
chemistry

experimental set-up



- Arepo and FLASH
- stochastic forcing (Ornstein-Uhlenbeck)
- self-gravity
- time-dependent chemistry (DVODE, standard variable-coefficient ordinary differential equation solver)
- cooling & heating processes
- gives you mathematically well defined boundary conditions
  --> good for statistical studies
- gives external radiation with TreeCol (a new approximative scheme to calculate column densities from the gravity solver)

chemical model 0

- 32 chemical species
  - 17 in instantaneous equilibrium:

H^-, H_2^+, H_3^+, CH^+, CH_2^+, OH^+, H_2O^+, H_3O^+, CO^+, HOC^+, O^-, C^- and O_2^+

  - 19 full non-equilibrium evolution

e^-, H^+, H, H_2, He, He^+, C, C^+, O, O^+, OH, H_2O, CO,

C_2, O_2, HCO^+, CH, CH_2 and CH_3^+

- 218 reactions
- various heating and cooling processes

long series of publications by Simon Glover and collaborators, e.g. Glover & Mac Low (2007ab), Glover, Federrath, Mac Low, Klessen (2010), Glover & Clark (2012, 2013), Clark & Clover (2012, 2013)

chemical model 1

Process	Reference(s)
Cooling:	
C fine structure lines	Atomic data – Silva & Viegas (2002)
	Collisional rates (H) – Abrahamsson, Krems & Dalgarno (2007)
	Collisional rates (H_2) – Schroder et al. (1991)
	Collisional rates (e^-) – Johnson et al. (1987)
	Collisional rates (H^+) – Roueff & Le Bourlot (1990)
C^+ fine structure lines	Atomic data – Silva & Viegas (2002)
	Collisional rates (H_2) – Flower & Launay (1977)
	Collisional rates (H, $T < 2000$ K) – Hollenbach & McKee (1989)
	Collisional rates (H, $T > 2000$ K) – Keenan et al. (1986)
	Collisional rates (e^-) – Wilson & Bell (2002)
O fine structure lines	Atomic data – Silva & Viegas (2002)
	Collisional rates (H) – Abrahamsson, Krems & Dalgarno (2007)
	Collisional rates (H_2) – see Glover & Jappsen (2007)
	Collisional rates (e^-) – Bell, Berrington & Thomas (1998)
	Collisional rates (H^+) – Pequignot (1990, 1996)
H_2 rovibrational lines	Le Bourlot, Pineau des Forêts & Flower (1999)
CO and H_2O rovibrational lines	Neufeld & Kaufman (1993); Neufeld, Lepp & Melnick (1995)
OH rotational lines	Pavlovski et al. (2002)
Gas-grain energy transfer	Hollenbach & McKee (1989)
Recombination on grains	Wolfire et al. (2003)
Atomic resonance lines	Sutherland & Dopita (1993)
H collisional ionization	Abel et al. (1997)
H_2 collisional dissociation	See Table B1
Compton cooling	Cen (1992)
Heating:	
Photoelectric effect	Bakes & Tielens (1994); Wolfire et al. (2003)
H_2 photodissociation	Black & Dalgarno (1977)
UV pumping of H_2	Burton, Hollenbach & Tielens (1990)
H_2 formation on dust grains	Hollenbach & McKee (1989)
Cosmic ray ionization	Goldsmith & Langer (1978)

(Glover, Federrath, Mac Low, Klessen, 2010, MNRS, 404, 2)

chemical model 2

Table B1. List of collisional gas-phase reactions included in our chemical model.

No.	Reaction	Rate coefficient	Notes	Ref.
1	$H + e^- \rightarrow H^- + \gamma$	$k_1 = \mathrm{dex}[-17.845 + 0.762 \log T + 0.1523(\log T)^2 - 0.03274(\log T)^3]$	$T \leqslant 6000$ K	1
		$= \mathrm{dex}[-16.420 + 0.1998(\log T)^2 - 5.447 \times 10^{-3}(\log T)^4 + 4.0415 \times 10^{-5}(\log T)^6]$	$T > 6000$ K	
2	$H^- + H \rightarrow H_2 + e^-$	$k_2 = 1.5 \times 10^{-9}$	$T \leqslant 300$ K	2
		$= 4.0 \times 10^{-9} T^{-0.17}$	$T > 300$ K	
3	$H + H^+ \rightarrow H_2^+ + \gamma$	$k_3 = \mathrm{dex}[-19.38 - 1.523 \log T + 1.118(\log T)^2 - 0.1269(\log T)^3]$		3
4	$H + H_2^+ \rightarrow H_2 + H^+$	$k_4 = 6.4 \times 10^{-10}$		4
5	$H^- + H^+ \rightarrow H + H$	$k_5 = 2.4 \times 10^{-6} T^{-1/2}(1.0 + T/20000)$		5
6	$H_2^+ + e^- \rightarrow H + H$	$k_6 = 1.0 \times 10^{-8}$	$T \leqslant 617$ K	6
		$= 1.32 \times 10^{-6} T^{-0.76}$	$T > 617$ K	
7	$H_2 + H^+ \rightarrow H_2^+ + H$	$k_7 = [-3.3232183 \times 10^{-7} + 3.3735382 \times 10^{-7} \ln T - 1.4491368 \times 10^{-7} (\ln T)^2 + 3.4172805 \times 10^{-8} (\ln T)^3 - 4.7813720 \times 10^{-9} (\ln T)^4 + 3.9731542 \times 10^{-10} (\ln T)^5 - 1.8171411 \times 10^{-11} (\ln T)^6 + 3.5311932 \times 10^{-13} (\ln T)^7] \times \exp\left(\frac{-21237.15}{T}\right)$		7
8	$H_2 + e^- \rightarrow H + H + e^-$	$k_8 = 3.73 \times 10^{-9} T^{0.1121} \exp\left(\frac{-99430}{T}\right)$		8
9	$H_2 + H \rightarrow H + H + H$	$k_{9,\mathrm{l}} = 6.67 \times 10^{-12} T^{1/2} \exp\left[-(1 + \frac{63590}{T})\right]$		9
		$k_{9,\mathrm{h}} = 3.52 \times 10^{-9} \exp\left(-\frac{43900}{T}\right)$		10
		$n_{\mathrm{cr,H}} = \mathrm{dex}\left[3.0 - 0.416 \log\left(\frac{T}{10000}\right) - 0.327 \left\{\log\left(\frac{T}{10000}\right)\right\}^2\right]$		10
10	$H_2 + H_2 \rightarrow H_2 + H + H$	$k_{10,\mathrm{l}} = \frac{5.996 \times 10^{-30} T^{4.1881}}{(1.0 + 6.761 \times 10^{-6} T)^{5.6881}} \exp\left(-\frac{54657.4}{T}\right)$		11
		$k_{10,\mathrm{h}} = 1.3 \times 10^{-9} \exp\left(-\frac{53300}{T}\right)$		12
		$n_{\mathrm{cr,H_2}} = \mathrm{dex}\left[4.845 - 1.3 \log\left(\frac{T}{10000}\right) + 1.62 \left\{\log\left(\frac{T}{10000}\right)\right\}^2\right]$		12
11	$H + e^- \rightarrow H^+ + e^- + e^-$	$k_{11} = \exp[-3.271396786 \times 10^1 + 1.35365560 \times 10^1 \ln T_e - 5.73932875 \times 10^0 (\ln T_e)^2 + 1.56315498 \times 10^0 (\ln T_e)^3 - 2.87705600 \times 10^{-1} (\ln T_e)^4 + 3.48255977 \times 10^{-2} (\ln T_e)^5 - 2.63197617 \times 10^{-3} (\ln T_e)^6 + 1.11954395 \times 10^{-4} (\ln T_e)^7 - 2.03914985 \times 10^{-6} (\ln T_e)^8]$		13
12	$H^+ + e^- \rightarrow H + \gamma$	$k_{12,\mathrm{A}} = 1.269 \times 10^{-13} \left(\frac{315614}{T}\right)^{1.503} \times \left[1.0 + \left(\frac{604625}{T}\right)^{0.470}\right]^{-1.923}$	Case A	14
		$k_{12,\mathrm{B}} = 2.753 \times 10^{-14} \left(\frac{315614}{T}\right)^{1.500} \times \left[1.0 + \left(\frac{115188}{T}\right)^{0.407}\right]^{-2.242}$	Case B	14
13	$H^- + e^- \rightarrow H + e^- + e^-$	$k_{13} = \exp[-1.801849334 \times 10^1 + 2.36085220 \times 10^0 \ln T_e - 2.82744300 \times 10^{-1} (\ln T_e)^2 + 1.62331664 \times 10^{-2} (\ln T_e)^3 - 3.36501203 \times 10^{-2} (\ln T_e)^4 + 1.17832978 \times 10^{-2} (\ln T_e)^5 - 1.65619470 \times 10^{-3} (\ln T_e)^6 + 1.06827520 \times 10^{-4} (\ln T_e)^7 - 2.63128581 \times 10^{-6} (\ln T_e)^8]$		13

(Glover, Federrath, Mac Low, Klessen, 2010, MNRS, 404, 2)

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Table B1. [illegible]

No.	Rea…
1	H +
2	H^-
3	H +
4	H +
5	H^-
6	H_2^+
7	H_2
8	H_2
9	H_2
10	H_2
11	H +
12	H^+
13	H^-

14	$H^- + H \rightarrow H + H + e^-$	$k_{14} = 2.5634 \times 10^{-9} T_e^{1.78186}$	$T_e \leqslant 0.1$ eV	13
		$= \exp[-2.0372609 \times 10^1$		
		$+ 1.13944933 \times 10^0 \ln T_e$		
		$- 1.4210135 \times 10^{-1} (\ln T_e)^2$		
		$+ 8.4644554 \times 10^{-3} (\ln T_e)^3$		
		$- 1.$[illegible]7641×10^{-3}[illegible]$\ln T_e)^4$		
		$+ 2.$[illegible]$\times 10^{-4}$[illegible]$\ln T_e)^5$		
		$+ 8.6639632 \times 10^{-5} (\ln T_e)^6$		
		$- 2.5850097 \times 10^{-5} (\ln T_e)^7$		
		$+ 2.4555012 \times 10^{-6} (\ln T_e)^8$		
		$- 8.0683825 \times 10^{-8} (\ln T_e)^9]$	$T_e > 0.1$ eV	
15	$H^- + H^+ \rightarrow H_2^+ + e^-$	$k_{15} = 6.9 \times 10^{-9} T^{-0.35}$	$T \leqslant 8000$ K	15
		$= 9.6 \times 10^{-7} T^{-0.90}$	$T > 8000$ K	
16	$He + e^- \rightarrow He^+ + e^- + e^-$	$k_{16} = \exp[-4.409864886 \times 10^1$		13
		$+ 2.391596563 \times 10^1 \ln T_e$		
		$- 1.07532302 \times 10^1 (\ln T_e)^2$		
		$+ 3.05803875 \times 10^0 (\ln T_e)^3$		
		$- 5.6851189 \times 10^{-1} (\ln T_e)^4$		
		$+ 6.79539123 \times 10^{-2} (\ln T_e)^5$		
		$- 5.0090561 \times 10^{-3} (\ln T_e)^6$		
		$+ 2.06723616 \times 10^{-4} (\ln T_e)^7$		
		$- 3.64916141 \times 10^{-6} (\ln T_e)^8]$		
17	$He^+ + e^- \rightarrow He + \gamma$	$k_{17,rr,A} = 10^{-11} T^{-0.5} [12.72 - 1.615 \log T$	Case A	16
		$- 0.3162 (\log T)^2 + 0.0493 (\log T)^3]$		
		$k_{17,rr,B} = 10^{-11} T^{-0.5} [11.19 - 1.676 \log T$	Case B	16
		$- 0.2852 (\log T)^2 + 0.04433 (\log T)^3]$		
		$k_{17,di} = 1.9 \times 10^{-3} T^{-1.5} \exp\left(-\frac{473421}{T}\right)$		
		$\times \left[1.0 + 0.3 \exp\left(-\frac{94684}{T}\right)\right]$		17
18	$He^+ + H \rightarrow He + H^+$	$k_{18} = 1.25 \times 10^{-15} \left(\frac{T}{300}\right)^{0.25}$		18
19	$He + H^+ \rightarrow He^+ + H$	$k_{19} = 1.26 \times 10^{-9} T^{-0.75} \exp\left(-\frac{127500}{T}\right)$	$T \leqslant 10000$ K	19
		$= 4.0 \times 10^{-37} T^{4.74}$	$T > 10000$ K	
20	$C^+ + e^- \rightarrow C + \gamma$	$k_{20} = 4.67 \times 10^{-12} \left(\frac{T}{300}\right)^{-0.6}$	$T \leqslant 7950$ K	20
		$= 1.23 \times 10^{-17} \left(\frac{T}{300}\right)^{2.49} \exp\left(\frac{21845.6}{T}\right)$	$7950 \text{ K} < T \leqslant 21140$ K	
		$= 9.62 \times 10^{-8} \left(\frac{T}{300}\right)^{-1.37} \exp\left(\frac{-115786.2}{T}\right)$	$T > 21140$ K	
21	$O^+ + e^- \rightarrow O + \gamma$	$k_{21} = 1.30 \times 10^{-10} T^{-0.64}$	$T \leqslant 400$ K	21
		$= 1.41 \times 10^{-10} T^{-0.66} + 7.4 \times 10^{-4} T^{-1.5}$		
		$\times \exp\left(-\frac{175000}{T}\right) [1.0 + 0.062 \times \exp\left(-\frac{145000}{T}\right)]$	$T > 400$ K	
22	$C + e^- \rightarrow C^+ + e^- + e^-$	$k_{22} = 6.85 \times 10^{-8} (0.193 + u)^{-1} u^{0.25} e^{-u}$	$u = 11.26/T_e$	22
23	$O + e^- \rightarrow O^+ + e^- + e^-$	$k_{23} = 3.59 \times 10^{-8} (0.073 + u)^{-1} u^{0.34} e^{-u}$	$u = 13.6/T_e$	22
24	$O^+ + H \rightarrow O + H^+$	$k_{24} = 4.99 \times 10^{-11} T^{0.405} + 7.54 \times 10^{-10} T^{-0.458}$		23
25	$O + H^+ \rightarrow O^+ + H$	$k_{25} = [1.08 \times 10^{-11} T^{0.517}$		24
		$+ 4.00 \times 10^{-10} T^{0.00669}] \exp\left(-\frac{227}{T}\right)$		
26	$O + He^+ \rightarrow O^+ + He$	$k_{26} = 4.991 \times 10^{-15} \left(\frac{T}{10000}\right)^{0.3794} \exp\left(-\frac{T}{1121000}\right)$		25
		$+ 2.780 \times 10^{-15} \left(\frac{T}{10000}\right)^{-0.2163} \exp\left(\frac{T}{815800}\right)$		
27	$C + H^+ \rightarrow C^+ + H$	$k_{27} = 3.9 \times 10^{-16} T^{0.213}$		24
28	$C^+ + H \rightarrow C + H^+$	$k_{28} = 6.08 \times 10^{-14} \left(\frac{T}{10000}\right)^{1.96} \exp\left(-\frac{170000}{T}\right)$		24
29	$C + He^+ \rightarrow C^+ + He$	$k_{29} = 8.58 \times 10^{-17} T^{0.757}$	$T \leqslant 200$ K	26
		$= 3.25 \times 10^{-17} T^{0.968}$	$200 < T \leqslant 2000$ K	
		$= 2.77 \times 10^{-19} T^{1.597}$	$T > 2000$ K	
30	$H_2 + He \rightarrow H + H + He$	$k_{30,l} = \mathrm{dex}[-27.029 + 3.801 \log(T) - 29487/T]$		27
		$k_{30,h} = \mathrm{dex}[-2.729 - 1.75 \log(T) - 23474/T]$		
		$n_{cr,He} = \mathrm{dex}\left[5.0792(1.0 - 1.23 \times 10^{-5}(T - 2000)\right]$		27
31	$OH + H \rightarrow O + H + H$	$k_{31} = 6.0 \times 10^{-9} \exp\left(-\frac{50900}{T}\right)$		28
32	$HOC^+ + H_2 \rightarrow HCO^+ + H_2$	$k_{32} = 3.8 \times 10^{-10}$		29
33	$HOC^+ + CO \rightarrow HCO^+ + CO$	$k_{33} = 4.0 \times 10^{-10}$		30
34	$C + H_2 \rightarrow CH + H$	$k_{34} = 6.64 \times 10^{-10} \exp\left(-\frac{11700}{T}\right)$		31
35	$CH + H \rightarrow C + H_2$	$k_{35} = 1.31 \times 10^{-10} \exp\left(-\frac{80}{T}\right)$		32

(Glover, Federrath, Mac Low, Klessen, 2010, MNRS, 404, 2)

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Table B1.

No.	Reaction	Rate coefficient	Notes	Ref.
14	$H^- + H \rightarrow H + H + e^-$	$k_{14} = 2.5634 \times 10^{-9} T_e^{1.78186}$	$T_e \leqslant 0.1$ eV	13
36	$CH + H_2 \rightarrow CH_2 + H$	$k_{36} = 5.46 \times 10^{-10} \exp\left(-\frac{1943}{T}\right)$		33
37	$CH + C \rightarrow C_2 + H$	$k_{37} = 6.59 \times 10^{-11}$		34
38	$CH + O \rightarrow CO + H$	$k_{38} = 6.6 \times 10^{-11}$	$T \leqslant 2000$ K	35
		$= 1.02 \times 10^{-10} \exp\left(-\frac{[illegible]}{T}\right)$	$T > 2000$ K	36
39	[illegible]	$k_{39} = [illegible] \times 10^{-11}$		37
40	$CH_2 + O \rightarrow CO + H + H$	$k_{40} = 1.33 \times 10^{-10}$		38
41	$CH_2 + O \rightarrow CO + H_2$	$k_{41} = 8.0 \times 10^{-11}$		39
42	$C_2 + O \rightarrow CO + C$	$k_{42} = 5.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.5}$	$T \leqslant 300$ K	40
		$= 5.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.757}$	$T > 300$ K	41
43	$O + H_2 \rightarrow OH + H$	$k_{43} = 3.14 \times 10^{-13} \left(\frac{T}{300}\right)^{2.7} \exp\left(-\frac{3150}{T}\right)$		42
44	$OH + H \rightarrow O + H_2$	$k_{44} = 6.99 \times 10^{-14} \left(\frac{T}{300}\right)^{2.8} \exp\left(-\frac{1950}{T}\right)$		43
45	$OH + H_2 \rightarrow H_2O + H$	$k_{45} = 2.05 \times 10^{-12} \left(\frac{T}{300}\right)^{1.52} \exp\left(-\frac{1736}{T}\right)$		44
46	$OH + C \rightarrow CO + H$	$k_{46} = 1.0 \times 10^{-10}$		34
47	$OH + O \rightarrow O_2 + H$	$k_{47} = 3.50 \times 10^{-11}$	$T \leqslant 261$ K	45
		$= 1.77 \times 10^{-11} \exp\left(\frac{178}{T}\right)$	$T > 261$ K	33
48	$OH + OH \rightarrow H_2O + H$	$k_{48} = 1.65 \times 10^{-12} \left(\frac{T}{300}\right)^{1.14} \exp\left(-\frac{50}{T}\right)$		34
49	$H_2O + H \rightarrow H_2 + OH$	$k_{49} = 1.59 \times 10^{-11} \left(\frac{T}{300}\right)^{1.2} \exp\left(-\frac{9610}{T}\right)$		46
50	$O_2 + H \rightarrow OH + O$	$k_{50} = 2.61 \times 10^{-10} \exp\left(-\frac{8156}{T}\right)$		33
51	$O_2 + H_2 \rightarrow OH + OH$	$k_{51} = 3.16 \times 10^{-10} \exp\left(-\frac{21890}{T}\right)$		47
52	$O_2 + C \rightarrow CO + O$	$k_{52} = 4.7 \times 10^{-11} \left(\frac{T}{300}\right)^{-0.34}$	$T \leqslant 295$ K	34
		$= 2.48 \times 10^{-12} \left(\frac{T}{300}\right)^{1.54} \exp\left(\frac{613}{T}\right)$	$T > 295$ K	33
53	$CO + H \rightarrow C + OH$	$k_{53} = 1.1 \times 10^{-10} \left(\frac{T}{300}\right)^{0.5} \exp\left(-\frac{77700}{T}\right)$		28
54	$H_2^+ + H_2 \rightarrow H_3^+ + H$	$k_{54} = 2.24 \times 10^{-9} \left(\frac{T}{300}\right)^{0.042} \exp\left(-\frac{T}{46600}\right)$		48
55	$H_3^+ + H \rightarrow H_2^+ + H_2$	$k_{55} = 7.7 \times 10^{-9} \exp\left(-\frac{17560}{T}\right)$		49
56	$C + H_2^+ \rightarrow CH^+ + H$	$k_{56} = 2.4 \times 10^{-9}$		28
57	$C + H_3^+ \rightarrow CH^+ + H_2$	$k_{57} = 2.0 \times 10^{-9}$		28
58	$C^+ + H_2 \rightarrow CH^+ + H$	$k_{58} = 1.0 \times 10^{-10} \exp\left(-\frac{4640}{T}\right)$		50
59	$CH^+ + H \rightarrow C^+ + H_2$	$k_{59} = 7.5 \times 10^{-10}$		51
60	$CH^+ + H_2 \rightarrow CH_2^+ + H$	$k_{60} = 1.2 \times 10^{-9}$		51
61	$CH^+ + O \rightarrow CO^+ + H$	$k_{61} = 3.5 \times 10^{-10}$		52
62	$CH_2 + H^+ \rightarrow CH^+ + H_2$	$k_{62} = 1.4 \times 10^{-9}$		28
63	$CH_2^+ + H \rightarrow CH^+ + H_2$	$k_{63} = 1.0 \times 10^{-9} \exp\left(-\frac{7080}{T}\right)$		28
64	$CH_2^+ + H_2 \rightarrow CH_3^+ + H$	$k_{64} = 1.6 \times 10^{-9}$		53
65	$CH_2^+ + O \rightarrow HCO^+ + H$	$k_{65} = 7.5 \times 10^{-10}$		28
66	$CH_3^+ + H \rightarrow CH_2^+ + H_2$	$k_{66} = 7.0 \times 10^{-10} \exp\left(-\frac{10560}{T}\right)$		28
67	$CH_3^+ + O \rightarrow HCO^+ + H_2$	$k_{67} = 4.0 \times 10^{-10}$		54
68	$C_2 + O^+ \rightarrow CO^+ + C$	$k_{68} = 4.8 \times 10^{-10}$		28
69	$O^+ + H_2 \rightarrow OH^+ + H$	$k_{69} = 1.7 \times 10^{-9}$		55
70	$O + H_2^+ \rightarrow OH^+ + H$	$k_{70} = 1.5 \times 10^{-9}$		28
71	$O + H_3^+ \rightarrow OH^+ + H_2$	$k_{71} = 8.4 \times 10^{-10}$		56
72	$OH + H_3^+ \rightarrow H_2O^+ + H_2$	$k_{72} = 1.3 \times 10^{-9}$		28
73	$OH + C^+ \rightarrow CO^+ + H$	$k_{73} = 7.7 \times 10^{-10}$		28
74	$OH^+ + H_2 \rightarrow H_2O^+ + H$	$k_{74} = 1.01 \times 10^{-9}$		57
75	$H_2O^+ + H_2 \rightarrow H_3O^+ + H$	$k_{75} = 6.4 \times 10^{-10}$		58
76	$H_2O + H_3^+ \rightarrow H_3O^+ + H_2$	$k_{76} = 5.9 \times 10^{-9}$		59
77	$H_2O + C^+ \rightarrow HCO^+ + H$	$k_{77} = 9.0 \times 10^{-10}$		60
78	$H_2O + C^+ \rightarrow HOC^+ + H$	$k_{78} = 1.8 \times 10^{-9}$		60
79	$H_3O^+ + C \rightarrow HCO^+ + H_2$	$k_{79} = 1.0 \times 10^{-11}$		28
80	$O_2 + C^+ \rightarrow CO^+ + O$	$k_{80} = 3.8 \times 10^{-10}$		53
81	$O_2 + C^+ \rightarrow CO + O^+$	$k_{81} = 6.2 \times 10^{-10}$		53
82	$O_2 + CH_2^+ \rightarrow HCO^+ + OH$	$k_{82} = 9.1 \times 10^{-10}$		53
83	$O_2^+ + C \rightarrow CO^+ + O$	$k_{83} = 5.2 \times 10^{-11}$		28
84	$CO + H_3^+ \rightarrow HOC^+ + H_2$	$k_{84} = 2.7 \times 10^{-11}$		61
85	$CO + H_3^+ \rightarrow HCO^+ + H_2$	$k_{85} = 1.7 \times 10^{-9}$		61
86	$HCO^+ + C \rightarrow CO + CH^+$	$k_{86} = 1.1 \times 10^{-9}$		28
87	$HCO^+ + H_2O \rightarrow CO + H_3O^+$	$k_{87} = 2.5 \times 10^{-9}$		62

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87	$HCO^+ + H_2O \rightarrow CO + H_3O^+$	$k_{87} = 2.5 \times 10^{-9}$	62
88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$	63
89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$	63
90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$	28
91	$CH_2 + H^+ \rightarrow CH_2^+ + H$	$k_{91} = 1.4 \times 10^{-9}$	28
92	$CH_2 + H$[illegible] $\rightarrow C$[illegible] $+$ [illegible]$e + H_2$	$k_{92} =$ [illegible]$.5 \times 10^{-}$[illegible]	28
93	$C_2 +$ [illegible]e[illegible] $\rightarrow C$[illegible] $+ C$[illegible] $+$ [illegible]e	$k_{93} =$ [illegible]6×10^{-9}	28
94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-}$[illegible]	28
95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$	28
96	$H_2O + H^+ \rightarrow H_2O^+ + H$	$k_{96} = 6.9 \times 10^{-9}$	64
97	$H_2O + He^+ \rightarrow OH + He + H^+$	$k_{97} = 2.04 \times 10^{-10}$	65
98	$H_2O + He^+ \rightarrow OH^+ + He + H$	$k_{98} = 2.86 \times 10^{-10}$	65
99	$H_2O + He^+ \rightarrow H_2O^+ + He$	$k_{99} = 6.05 \times 10^{-11}$	65
100	$O_2 + H^+ \rightarrow O_2^+ + H$	$k_{100} = 2.0 \times 10^{-9}$	64
101	$O_2 + He^+ \rightarrow O_2^+ + He$	$k_{101} = 3.3 \times 10^{-11}$	66
102	$O_2 + He^+ \rightarrow O^+ + O + He$	$k_{102} = 1.1 \times 10^{-9}$	66
103	$O_2^+ + C \rightarrow O_2 + C^+$	$k_{103} = 5.2 \times 10^{-11}$	28
104	$CO + He^+ \rightarrow C^+ + O + He$	$k_{104} = 1.4 \times 10^{-9} \left(\frac{T}{300}\right)^{-0.5}$	67
105	$CO + He^+ \rightarrow C + O^+ + He$	$k_{105} = 1.4 \times 10^{-16} \left(\frac{T}{300}\right)^{-0.5}$	67
106	$CO^+ + H \rightarrow CO + H^+$	$k_{106} = 7.5 \times 10^{-10}$	68
107	$C^- + H^+ \rightarrow C + H$	$k_{107} = 2.3 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	28
108	$O^- + H^+ \rightarrow O + H$	$k_{108} = 2.3 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	28
109	$He^+ + H^- \rightarrow He + H$	$k_{109} = 2.32 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.52} \exp\left(\frac{T}{22400}\right)$	69
110	$H_3^+ + e^- \rightarrow H_2 + H$	$k_{110} = 2.34 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.52}$	70
111	$H_3^+ + e^- \rightarrow H + H + H$	$k_{111} = 4.36 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.52}$	70
112	$CH^+ + e^- \rightarrow C + H$	$k_{112} = 7.0 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	71
113	$CH_2^+ + e^- \rightarrow CH + H$	$k_{113} = 1.6 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.6}$	72
114	$CH_2^+ + e^- \rightarrow C + H + H$	$k_{114} = 4.03 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.6}$	72
115	$CH_2^+ + e^- \rightarrow C + H_2$	$k_{115} = 7.68 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.6}$	72
116	$CH_3^+ + e^- \rightarrow CH_2 + H$	$k_{116} = 7.75 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	73
117	$CH_3^+ + e^- \rightarrow CH + H_2$	$k_{117} = 1.95 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	73
118	$CH_3^+ + e^- \rightarrow CH + H + H$	$k_{118} = 2.0 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.4}$	28
119	$OH^+ + e^- \rightarrow O + H$	$k_{119} = 6.3 \times 10^{-9} \left(\frac{T}{300}\right)^{-0.48}$	74
120	$H_2O^+ + e^- \rightarrow O + H + H$	$k_{120} = 3.05 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	75
121	$H_2O^+ + e^- \rightarrow O + H_2$	$k_{121} = 3.9 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	75
122	$H_2O^+ + e^- \rightarrow OH + H$	$k_{122} = 8.6 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	75
123	$H_3O^+ + e^- \rightarrow H + H_2O$	$k_{123} = 1.08 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	76
124	$H_3O^+ + e^- \rightarrow OH + H_2$	$k_{124} = 6.02 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	76
125	$H_3O^+ + e^- \rightarrow OH + H + H$	$k_{125} = 2.58 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	76
126	$H_3O^+ + e^- \rightarrow O + H + H_2$	$k_{126} = 5.6 \times 10^{-9} \left(\frac{T}{300}\right)^{-0.5}$	76
127	$O_2^+ + e^- \rightarrow O + O$	$k_{127} = 1.95 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.7}$	77
128	$CO^+ + e^- \rightarrow C + O$	$k_{128} = 2.75 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.55}$	78
129	$HCO^+ + e^- \rightarrow CO + H$	$k_{129} = 2.76 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.64}$	79
130	$HCO^+ + e^- \rightarrow OH + C$	$k_{130} = 2.4 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.64}$	79
131	$HOC^+ + e^- \rightarrow CO + H$	$k_{131} = 1.1 \times 10^{-7} \left(\frac{T}{300}\right)^{-1.0}$	28
132	$H^- + C \rightarrow CH + e^-$	$k_{132} = 1.0 \times 10^{-9}$	28
133	$H^- + O \rightarrow OH + e^-$	$k_{133} = 1.0 \times 10^{-9}$	28
134	$H^- + OH \rightarrow H_2O + e^-$	$k_{134} = 1.0 \times 10^{-10}$	28
135	$C^- + H \rightarrow CH + e^-$	$k_{135} = 5.0 \times 10^{-10}$	28
136	$C^- + H_2 \rightarrow CH_2 + e^-$	$k_{136} = 1.0 \times 10^{-13}$	28
137	$C^- + O \rightarrow CO + e^-$	$k_{137} = 5.0 \times 10^{-10}$	28
138	$O^- + H \rightarrow OH + e^-$	$k_{138} = 5.0 \times 10^{-10}$	28
139	$O^- + H_2 \rightarrow H_2O + e^-$	$k_{139} = 7.0 \times 10^{-10}$	28
140	$O^- + C \rightarrow CO + e^-$	$k_{140} = 5.0 \times 10^{-10}$	28

(Glover, Federrath, Mac Low, Klessen, 2010, MNRAS, 404, 2)

chemical model 2

(Glover, Federrath, Mac Low, Klessen, 2010, MNRS, 404, 2)

No.	Reaction	Rate coefficient	Notes	Ref.
88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$		63
89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$		63
90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$		28
91	$CH_2 + H^+ \rightarrow CH_2^+ + H$	$k_{91} = 1.4 \times 10^{-9}$		28
94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-9}$		28
95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$		28
96	$H_2O + H^+ \rightarrow H_2O^+ + H$	$k_{96} = 6.9 \times 10^{-9}$		64
97	$H_2O + He^+ \rightarrow OH + He + H^+$	$k_{97} = 2.04 \times 10^{-10}$		65
129	$HCO^+ + e^- \rightarrow CO + H$	$k_{129} = 2.76 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.64}$		79
130	$HCO^+ + e^- \rightarrow OH + C$	$k_{130} = 2.4 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.64}$		79
131	$HOC^+ + e^- \rightarrow CO + H$	$k_{131} = 1.1 \times 10^{-7} \left(\frac{T}{300}\right)^{-1.0}$		28
132	$H^- + C \rightarrow CH + e^-$	$k_{132} = 1.0 \times 10^{-9}$		28
133	$H^- + O \rightarrow OH + e^-$	$k_{133} = 1.0 \times 10^{-9}$		28
134	$H^- + OH \rightarrow H_2O + e^-$	$k_{134} = 1.0 \times 10^{-10}$		28
135	$C^- + H \rightarrow CH + e^-$	$k_{135} = 5.0 \times 10^{-10}$		28
136	$C^- + H_2 \rightarrow CH_2 + e^-$	$k_{136} = 1.0 \times 10^{-13}$		28
137	$C^- + O \rightarrow CO + e^-$	$k_{137} = 5.0 \times 10^{-10}$		28
138	$O^- + H \rightarrow OH + e^-$	$k_{138} = 5.0 \times 10^{-10}$		28
139	$O^- + H_2 \rightarrow H_2O + e^-$	$k_{139} = 7.0 \times 10^{-10}$		28
140	$O^- + C \rightarrow CO + e^-$	$k_{140} = 5.0 \times 10^{-10}$		28

No.	Reaction	Rate coefficient	Notes	Ref.
142	$C + e^- \rightarrow C^- + \gamma$	$k_{142} = 2.25 \times 10^{-15}$		81
143	$C + H \rightarrow CH + \gamma$	$k_{143} = 1.0 \times 10^{-17}$		82
144	$C + H_2 \rightarrow CH_2 + \gamma$	$k_{144} = 1.0 \times 10^{-17}$		82
145	$C + C \rightarrow C_2 + \gamma$	$k_{145} = 4.36 \times 10^{-18} \left(\frac{T}{300}\right)^{0.35} \exp\left(-\frac{161.3}{T}\right)$		83
146	$C + O \rightarrow CO + \gamma$	$k_{146} = 2.1 \times 10^{-19}$	$T \leqslant 300$ K	84
		$= 3.09 \times 10^{-17} \left(\frac{T}{300}\right)^{0.33} \exp\left(-\frac{1629}{T}\right)$	$T > 300$ K	85
147	$C^+ + H \rightarrow CH^+ + \gamma$	$k_{147} = 4.46 \times 10^{-16} T^{-0.5} \exp\left(-\frac{4.93}{T^{2/3}}\right)$		86
148	$C^+ + H_2 \rightarrow CH_2^+ + \gamma$	$k_{148} = 4.0 \times 10^{-16} \left(\frac{T}{300}\right)^{-0.2}$		87
149	$C^+ + O \rightarrow CO^+ + \gamma$	$k_{149} = 2.5 \times 10^{-18}$	$T \leqslant 300$ K	84
		$= 3.14 \times 10^{-18} \left(\frac{T}{300}\right)^{-0.15} \exp\left(\frac{68}{T}\right)$	$T > 300$ K	85
150	$O + e^- \rightarrow O^- + \gamma$	$k_{150} = 1.5 \times 10^{-15}$		28
151	$O + H \rightarrow OH + \gamma$	$k_{151} = 9.9 \times 10^{-19} \left(\frac{T}{300}\right)^{-0.38}$		28
152	$O + O \rightarrow O_2 + \gamma$	$k_{152} = 4.9 \times 10^{-20} \left(\frac{T}{300}\right)^{1.58}$		82
153	$OH + H \rightarrow H_2O + \gamma$	$k_{153} = 5.26 \times 10^{-18} \left(\frac{T}{300}\right)^{-5.22} \exp\left(-\frac{90}{T}\right)$		88
154	$H + H + H \rightarrow H_2 + H$	$k_{154} = 1.32 \times 10^{-32} \left(\frac{T}{300}\right)^{-0.38}$	$T \leqslant 300$ K	89
		$= 1.32 \times 10^{-32} \left(\frac{T}{300}\right)^{-1.0}$	$T > 300$ K	90
155	$H + H + H_2 \rightarrow H_2 + H_2$	$k_{155} = 2.8 \times 10^{-31} T^{-0.6}$		91
156	$H + H + He \rightarrow H_2 + He$	$k_{156} = 6.9 \times 10^{-32} T^{-0.4}$		92
157	$C + C + M \rightarrow C_2 + M$	$k_{157} = 5.99 \times 10^{-33} \left(\frac{T}{5000}\right)^{-1.6}$	$T \leqslant 5000$ K	93
		$= 5.99 \times 10^{-33} \left(\frac{T}{5000}\right)^{-0.64} \exp\left(\frac{5255}{T}\right)$	$T > 5000$ K	94
158	$C + O + M \rightarrow CO + M$	$k_{158} = 6.16 \times 10^{-29} \left(\frac{T}{300}\right)^{-3.08}$	$T \leqslant 2000$ K	35
		$= 2.14 \times 10^{-29} \left(\frac{T}{300}\right)^{-3.08} \exp\left(\frac{2114}{T}\right)$	$T > 2000$ K	67
159	$C^+ + O + M \rightarrow CO^+ + M$	$k_{159} = 100 \times k_{210}$		67
160	$C + O^+ + M \rightarrow CO^+ + M$	$k_{160} = 100 \times k_{210}$		67
161	$O + H + M \rightarrow OH + M$	$k_{161} = 4.33 \times 10^{-32} \left(\frac{T}{300}\right)^{-1.0}$		43
162	$OH + H + M \rightarrow H_2O + M$	$k_{162} = 2.56 \times 10^{-31} \left(\frac{T}{300}\right)^{-2.0}$		35
163	$O + O + M \rightarrow O_2 + M$	$k_{163} = 9.2 \times 10^{-34} \left(\frac{T}{300}\right)^{-1.0}$		37
164	$O + CH \rightarrow HCO^+ + e^-$	$k_{164} = 2.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.44}$		95
165	$H + H(s) \rightarrow H_2$	$k_{165} = 3.0 \times 10^{-18} T^{0.5} f_A [1.0 + 0.04(T + T_d)^{0.5} + 0.002\,T + 8 \times 10^{-6} T^2]^{-1}$	$f_A = \left[1.0 + 10^4 \exp\left(-\frac{600}{T_d}\right)\right]^{-1}$	96

chemical model 2

No.	Reaction	Rate coefficient	Ref.
88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$	63
89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$	63
90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$	28
91	[illegible]	[illegible]	28
92	[illegible]	[illegible]	28
93	[illegible]	[illegible]	28
94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-9}$	28
95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$	28
96	$H_2O + H^+ \rightarrow H_2O^+ + H$	$k_{96} = 6.9 \times 10^{-9}$	64
97	$H_2O + He^+ \rightarrow OH + He + H^+$	$k_{97} = 2.04 \times 10^{-10}$	65

Table B2. List of photochemical reactions included in our chemical model

No.	Reaction	Optically thin rate (s^{-1})	γ	Ref.
166	$H^- + \gamma \rightarrow H + e^-$	$R_{166} = 7.1 \times 10^{-7}$	0.5	1
167	$H_2^+ + \gamma \rightarrow H + H^+$	$R_{167} = 1.1 \times 10^{-9}$	1.9	2
168	$H_2 + \gamma \rightarrow H + H$	$R_{168} = 5.6 \times 10^{-11}$	See §2.2	3
169	$H_3^+ + \gamma \rightarrow H_2 + H^+$	$R_{169} = 4.9 \times 10^{-13}$	1.8	4
170	$H_3^+ + \gamma \rightarrow H_2^+ + H$	$R_{170} = 4.9 \times 10^{-13}$	2.3	4
171	$C + \gamma \rightarrow C^+ + e^-$	$R_{171} = 3.1 \times 10^{-10}$	3.0	5
172	$C^- + \gamma \rightarrow C + e^-$	$R_{172} = 2.4 \times 10^{-7}$	0.9	6
173	$CH + \gamma \rightarrow C + H$	$R_{173} = 8.7 \times 10^{-10}$	1.2	7
174	$CH + \gamma \rightarrow CH^+ + e^-$	$R_{174} = 7.7 \times 10^{-10}$	2.8	8
175	$CH^+ + \gamma \rightarrow C + H^+$	$R_{175} = 2.6 \times 10^{-10}$	2.5	7
176	$CH_2 + \gamma \rightarrow CH + H$	$R_{176} = 7.1 \times 10^{-10}$	1.7	7
177	$CH_2 + \gamma \rightarrow CH_2^+ + e^-$	$R_{177} = 5.9 \times 10^{-10}$	2.3	6
178	$CH_2^+ + \gamma \rightarrow CH^+ + H$	$R_{178} = 4.6 \times 10^{-10}$	1.7	9
179	$CH_3^+ + \gamma \rightarrow CH_2^+ + H$	$R_{179} = 1.0 \times 10^{-9}$	1.7	6
180	$CH_3^+ + \gamma \rightarrow CH^+ + H_2$	$R_{180} = 1.0 \times 10^{-9}$	1.7	6
181	$C_2 + \gamma \rightarrow C + C$	$R_{181} = 1.5 \times 10^{-10}$	2.1	7
182	$O^- + \gamma \rightarrow O + e^-$	$R_{182} = 2.4 \times 10^{-7}$	0.5	6
183	$OH + \gamma \rightarrow O + H$	$R_{183} = 3.7 \times 10^{-10}$	1.7	10
184	$OH + \gamma \rightarrow OH^+ + e^-$	$R_{184} = 1.6 \times 10^{-12}$	3.1	6
185	$OH^+ + \gamma \rightarrow O + H^+$	$R_{185} = 1.0 \times 10^{-12}$	1.8	4
186	$H_2O + \gamma \rightarrow OH + H$	$R_{186} = 6.0 \times 10^{-10}$	1.7	11
187	$H_2O + \gamma \rightarrow H_2O^+ + e^-$	$R_{187} = 3.2 \times 10^{-11}$	3.9	8
188	$H_2O^+ + \gamma \rightarrow H_2^+ + O$	$R_{188} = 5.0 \times 10^{-11}$	See §2.2	12
189	$H_2O^+ + \gamma \rightarrow H^+ + OH$	$R_{189} = 5.0 \times 10^{-11}$	See §2.2	12
190	$H_2O^+ + \gamma \rightarrow O^+ + H_2$	$R_{190} = 5.0 \times 10^{-11}$	See §2.2	12
191	$H_2O^+ + \gamma \rightarrow OH^+ + H$	$R_{191} = 1.5 \times 10^{-10}$	See §2.2	12
192	$H_3O^+ + \gamma \rightarrow H^+ + H_2O$	$R_{192} = 2.5 \times 10^{-11}$	See §2.2	12
193	$H_3O^+ + \gamma \rightarrow H_2^+ + OH$	$R_{193} = 2.5 \times 10^{-11}$	See §2.2	12
194	$H_3O^+ + \gamma \rightarrow H_2O^+ + H$	$R_{194} = 7.5 \times 10^{-12}$	See §2.2	12
195	$H_3O^+ + \gamma \rightarrow OH^+ + H_2$	$R_{195} = 2.5 \times 10^{-11}$	See §2.2	12
196	$O_2 + \gamma \rightarrow O_2^+ + e^-$	$R_{196} = 5.6 \times 10^{-11}$	3.7	7
197	$O_2 + \gamma \rightarrow O + O$	$R_{197} = 7.0 \times 10^{-10}$	1.8	7
198	$CO + \gamma \rightarrow C + O$	$R_{198} = 2.0 \times 10^{-10}$	See §2.2	13

(Glover, Federrath, Mac Low, Klessen, 2010, MNRS, 404, 2)

chemical model 2

88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$	63
89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$	63
90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$	28
94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-9}$	28
95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$	28
96	$H_2O + H^+ \rightarrow H_2O^+ + H$	$k_{96} = 6.9 \times 10^{-9}$	64
97	$H_2O + He^+ \rightarrow OH + He + H^+$	$k_{97} = 2.04 \times 10^{-10}$	65

Table B2. List of photochemical reactions included in our chemical model

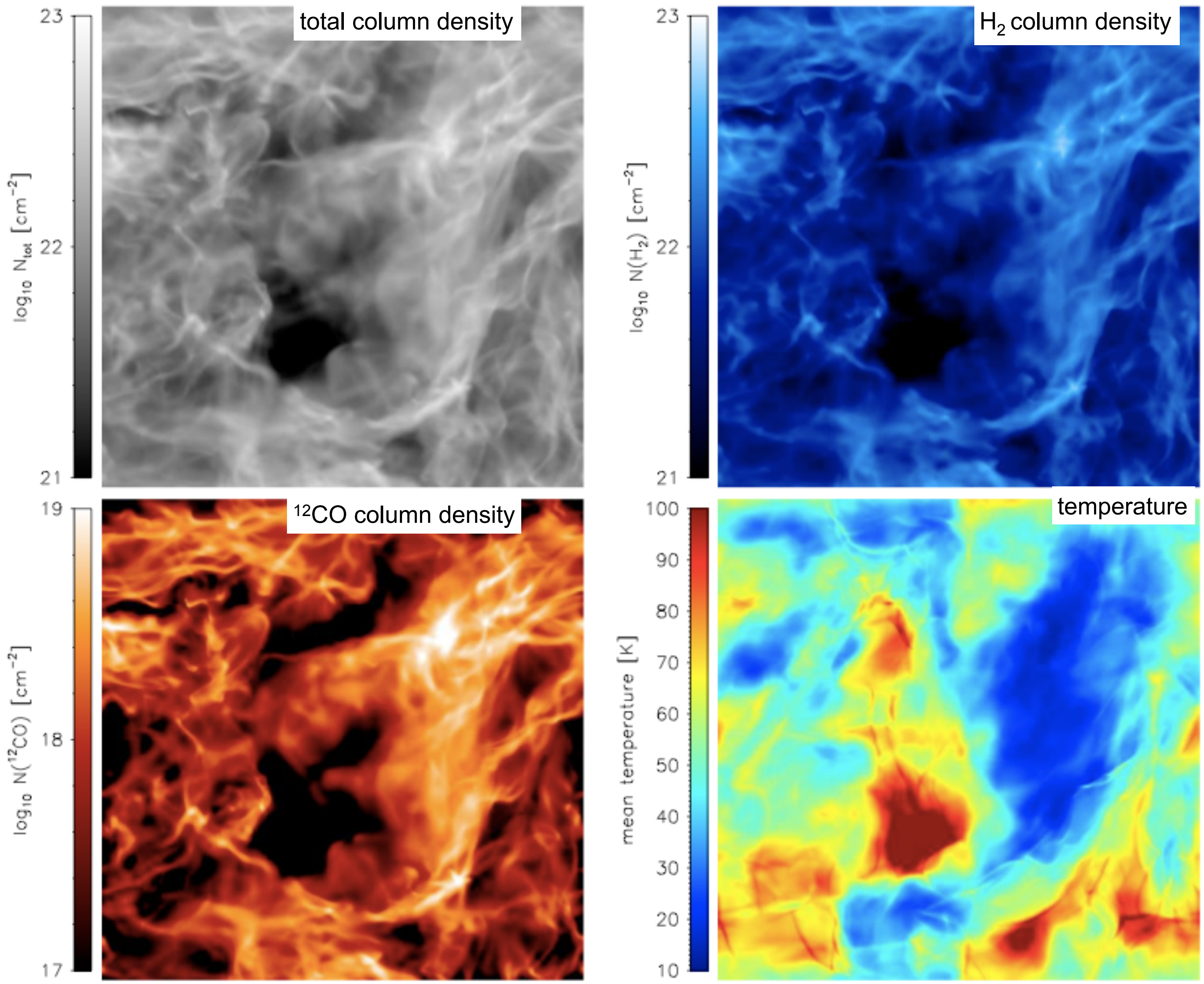
No.	Reaction	Optically thin rate (s^{-1})	γ	Ref.
166	$H^- + \gamma \rightarrow H + e^-$	$R_{166} = 7.1 \times 10^{-7}$	0.5	1
167	$H_2^+ + \gamma \rightarrow H + H^+$	$R_{167} = 1.1 \times 10^{-9}$	1.9	2
168	$H_2 + \gamma \rightarrow H + H$	$R_{168} = 5.6 \times 10^{-11}$	See §2.2	3
169	$H_3^+ + \gamma \rightarrow H_2 + H^+$	$R_{169} = 4.9 \times 10^{-13}$	1.8	4
170	$H_3^+ + \gamma \rightarrow H_2^+ + H$	$R_{170} = 4.9 \times 10^{-13}$	2.3	4
171	$C + \gamma \rightarrow C^+ + e^-$	[illegible]	[illegible]	[illegible]
172	$C^- + \gamma$ [illegible]			
173	$CH + \gamma$ [illegible]			
174	$CH + \gamma$ [illegible]			
175	$CH^+ + \gamma$ [illegible]			
176	$CH_2 + \gamma$ [illegible]			
177	$CH_2 + \gamma$ [illegible]			
178	$CH_2^+ + \gamma$ [illegible]			
179	$CH_3^+ + \gamma$ [illegible]			
180	$CH_3^+ + \gamma$ [illegible]			
181	$C_2 + \gamma$ [illegible]			
182	$O^- + \gamma$ [illegible]			
183	$OH + \gamma$ [illegible]			
184	$OH + \gamma$ [illegible]			
185	$OH^+ + \gamma$ [illegible]			
186	$H_2O + \gamma$ [illegible]			
187	$H_2O + \gamma$ [illegible]			
188	$H_2O^+ +$ [illegible]			
189	$H_2O^+ +$ [illegible]			
190	$H_2O^+ +$ [illegible]			
191	$H_2O^+ +$ [illegible]			
192	$H_3O^+ +$ [illegible]			
193	$H_3O^+ +$ [illegible]			
194	$H_3O^+ +$ [illegible]			
195	$H_3O^+ +$ [illegible]			
196	$O_2 + \gamma$ [illegible]			
197	$O_2 + \gamma \rightarrow O + O$	$R_{197} = 7.0 \times 10^{-10}$	1.8	7
198	$CO + \gamma \rightarrow C + O$	$R_{198} = 2.0 \times 10^{-10}$	See §2.2	13

Table B3. List of reactions included in our chemical model that involve cosmic rays or cosmic-ray induced UV emission

No.	Reaction	Rate ($s^{-1} \zeta_H^{-1}$)	Ref.
199	$H + c.r. \rightarrow H^+ + e^-$	$R_{199} = 1.0$	—
200	$He + c.r. \rightarrow He^+ + e^-$	$R_{200} = 1.1$	1
201	$H_2 + c.r. \rightarrow H^+ + H + e^-$	$R_{201} = 0.037$	1
202	$H_2 + c.r. \rightarrow H + H$	$R_{202} = 0.22$	1
203	$H_2 + c.r. \rightarrow H^+ + H^-$	$R_{203} = 6.5 \times 10^{-4}$	1
204	$H_2 + c.r. \rightarrow H_2^+ + e^-$	$R_{204} = 2.0$	1
205	$C + c.r. \rightarrow C^+ + e^-$	$R_{205} = 3.8$	1
206	$O + c.r. \rightarrow O^+ + e^-$	$R_{206} = 5.7$	1
207	$CO + c.r. \rightarrow CO^+ + e^-$	$R_{207} = 6.5$	1
208	$C + \gamma_{c.r.} \rightarrow C^+ + e^-$	$R_{208} = 2800$	2
209	$CH + \gamma_{c.r.} \rightarrow C + H$	$R_{209} = 4000$	3
210	$CH^+ + \gamma_{c.r.} \rightarrow C^+ + H$	$R_{210} = 960$	3
211	$CH_2 + \gamma_{c.r.} \rightarrow CH_2^+ + e^-$	$R_{211} = 2700$	1
212	$CH_2 + \gamma_{c.r.} \rightarrow CH + H$	$R_{212} = 2700$	1
213	$C_2 + \gamma_{c.r.} \rightarrow C + C$	$R_{213} = 1300$	3
214	$OH + \gamma_{c.r.} \rightarrow O + H$	$R_{214} = 2800$	3
215	$H_2O + \gamma_{c.r.} \rightarrow OH + H$	$R_{215} = 5300$	3
216	$O_2 + \gamma_{c.r.} \rightarrow O + O$	$R_{216} = 4100$	3
217	$O_2 + \gamma_{c.r.} \rightarrow O_2^+ + e^-$	$R_{217} = 640$	3
218	$CO + \gamma_{c.r.} \rightarrow C + O$	$R_{218} = 0.21 T^{1/2} x_{H_2} x_{CO}^{-1/2}$	4

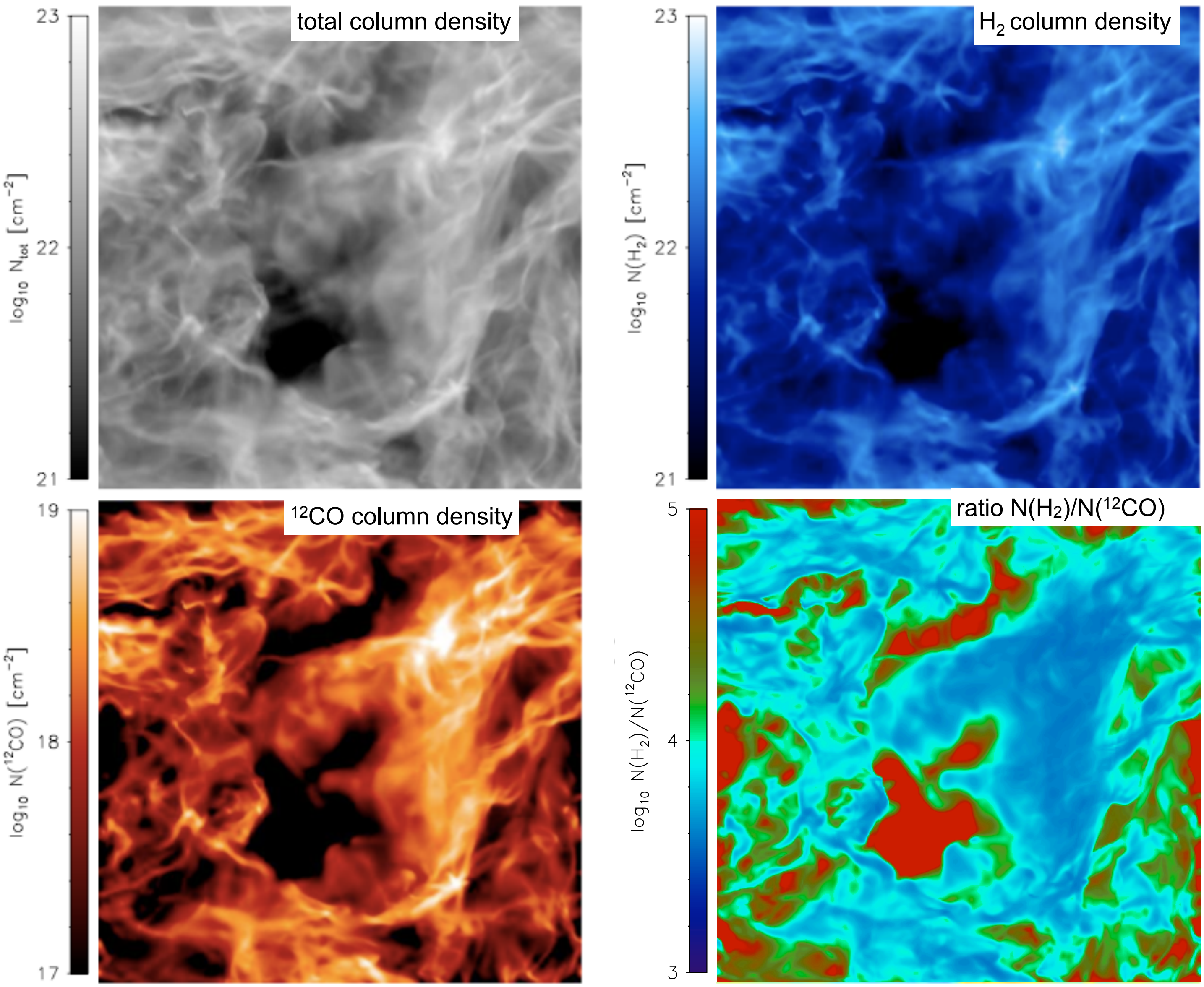
(Glover, Federrath, Mac Low, Klessen, 2010, MNRS, 404, 2)

effects of chemistry



(Glover et al. 2010)

effects of chemistry



(Glover et al. 2010)

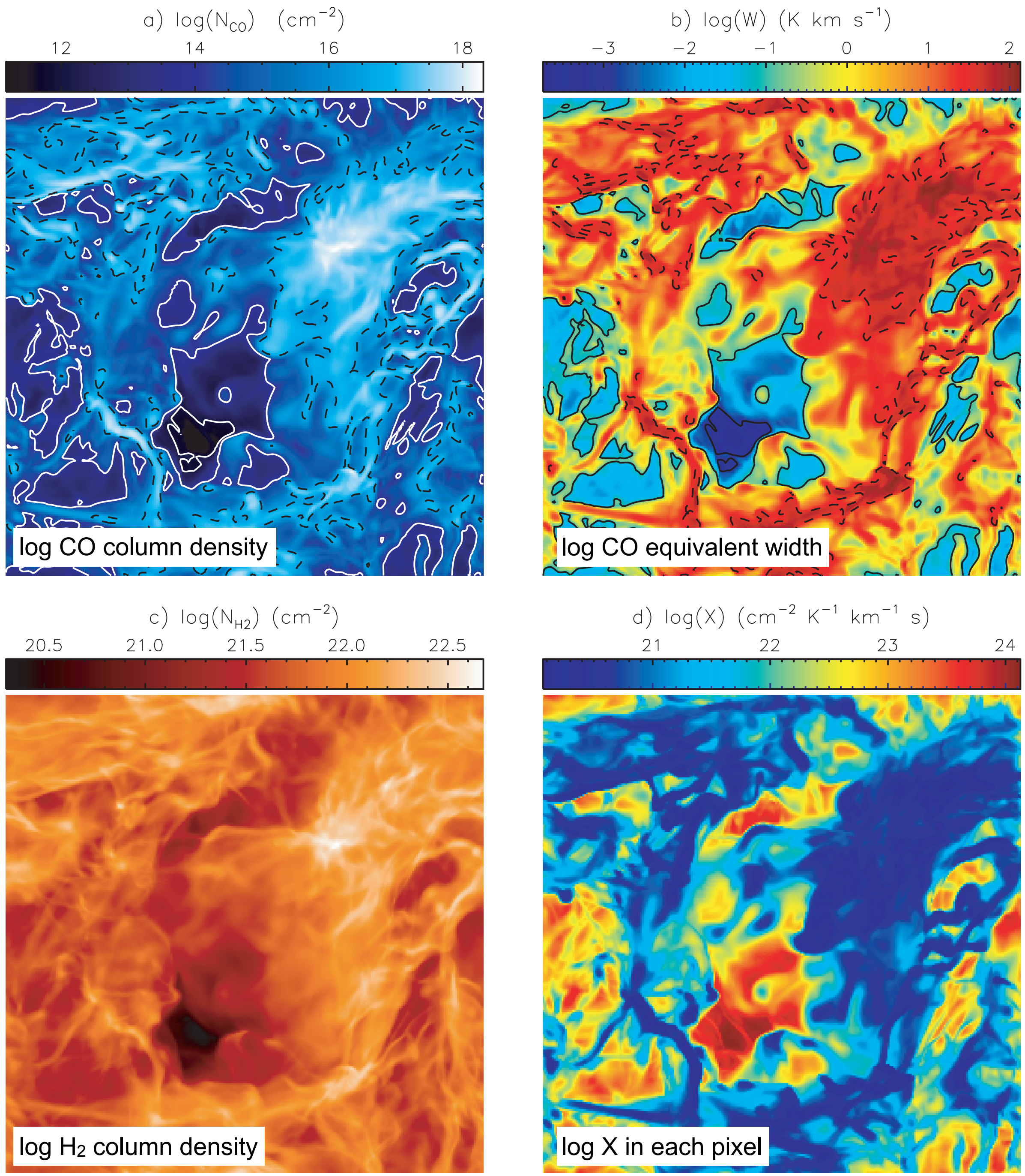
Xco factor

x-factor

- conversion rate between H_2 column density and CO emission (equivalent width W)

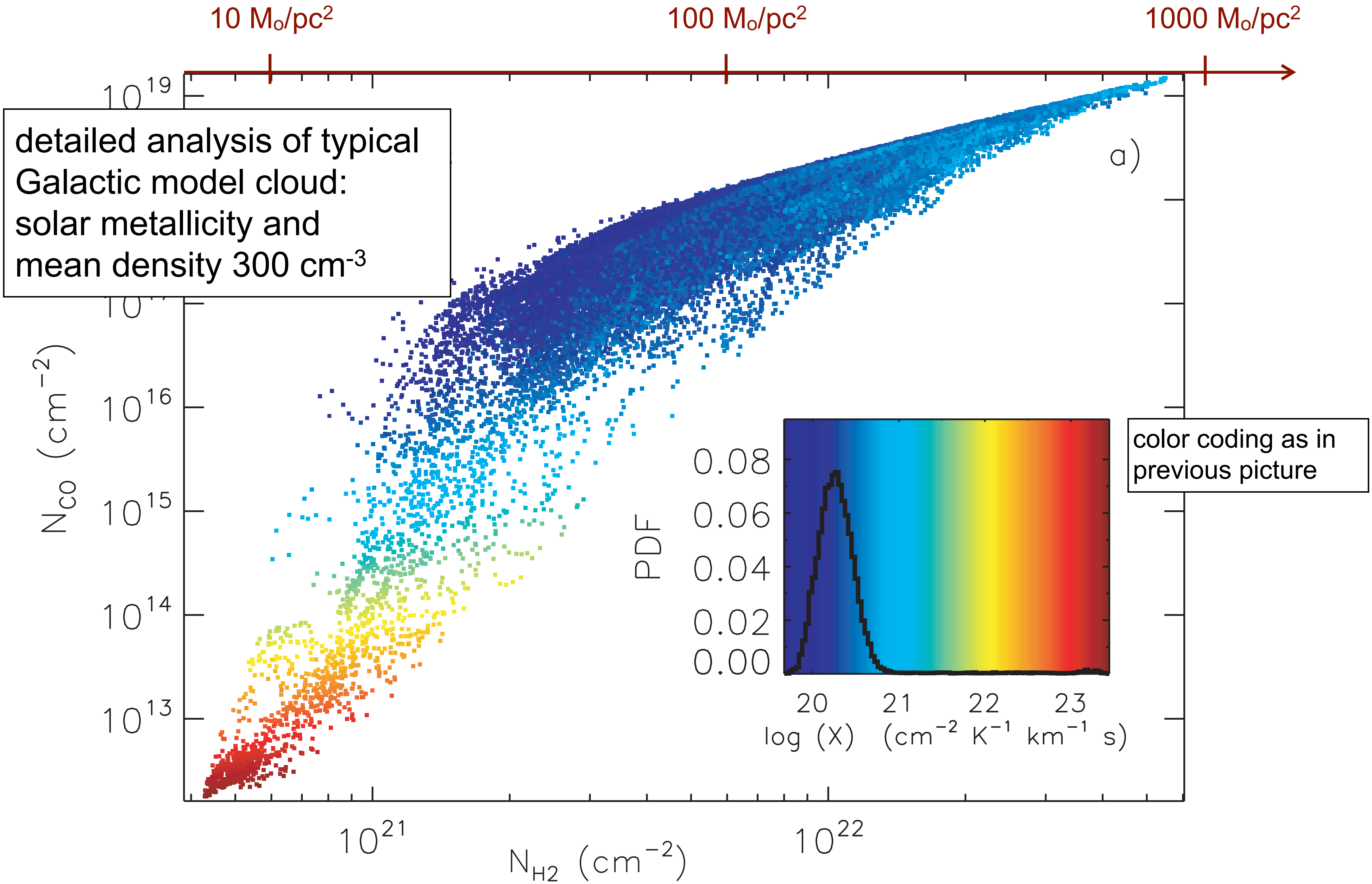
$$X = \frac{N_{H_2}}{W} \ (\mathrm{cm^{-2}\,K^{-1}\,km^{-1}\,s})$$

- most mass H_2 determinations depend on X*!*
- in Milky Way X ~ few x 10^{22} $\mathrm{cm^{-2}\,K^{-1}\,km^{-1}\,s}$ ~ const.
- why is it constant?
- how does it vary with environmental condition?
  - metallicity
  - density, radiation field, etc.
    ("normal" gal. vs star burst)



(Shetty, Glover, Dullemond, Klessen 2011)

Figure 4. Images of (a) N_{CO}, (b) W, (c) N_{H_2} and (d) the X factor of model n300-Z03. Each side has a length of 20 pc. In (a) and (b), solid contours indicate $\log(N_{CO}) = 12$, 14 and $\log(W) = -3, -1$; dashed contours are $\log(N_{CO}) = 16.5$ and $\log(W) = 1.5$ (see the text and Fig. 2d).



(Shetty, Glover, Dullemond, Klessen 2011)

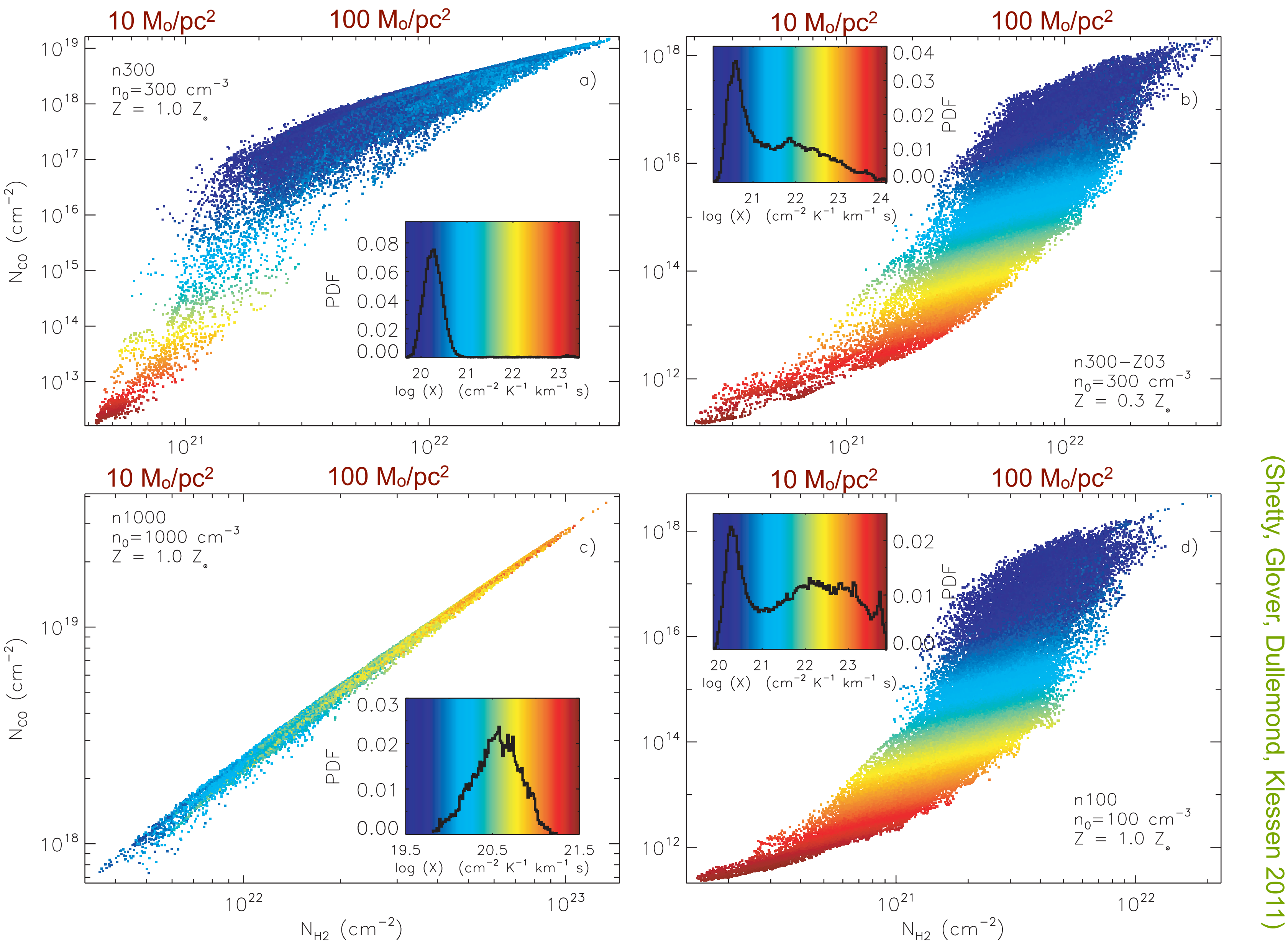
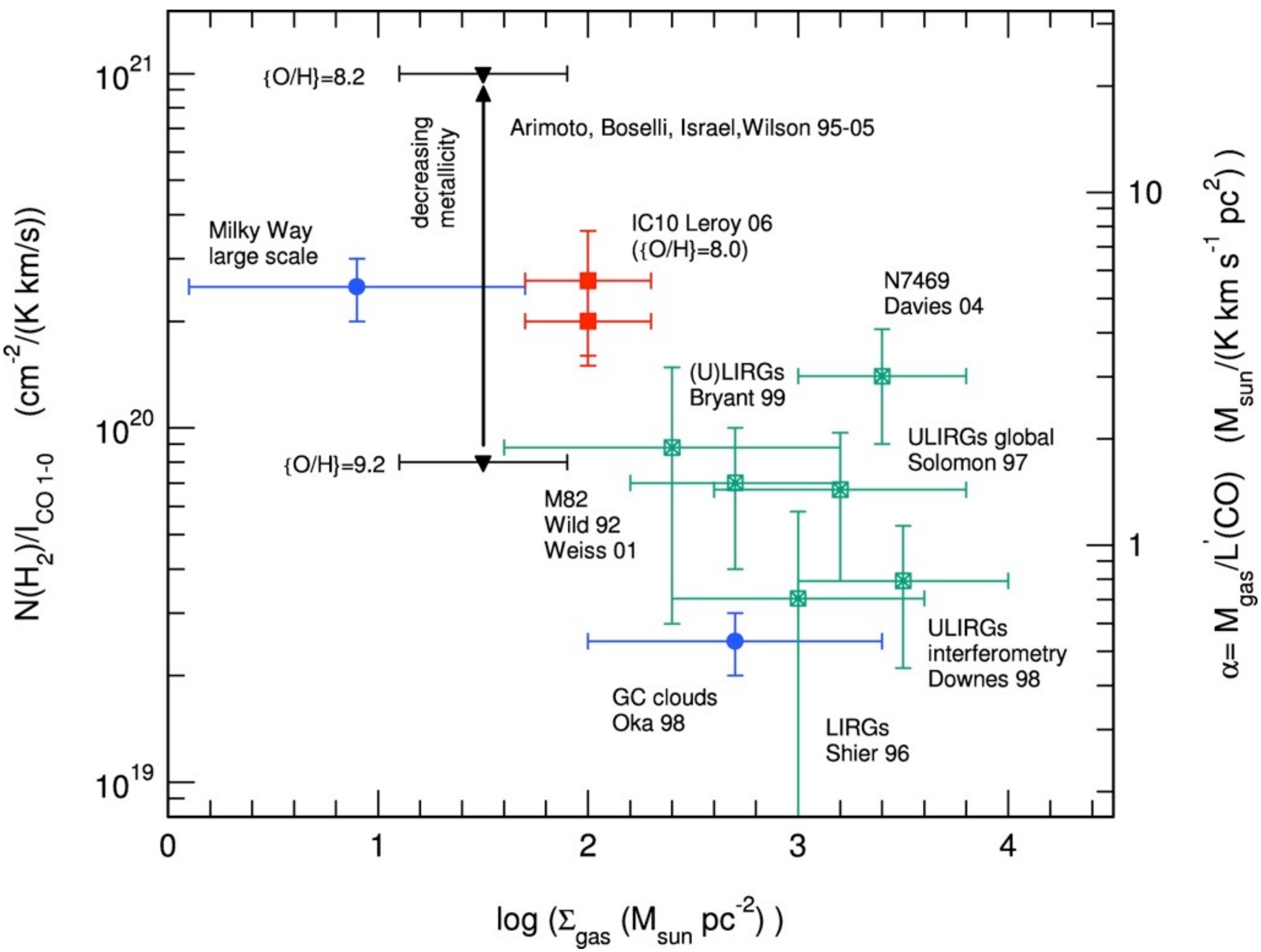


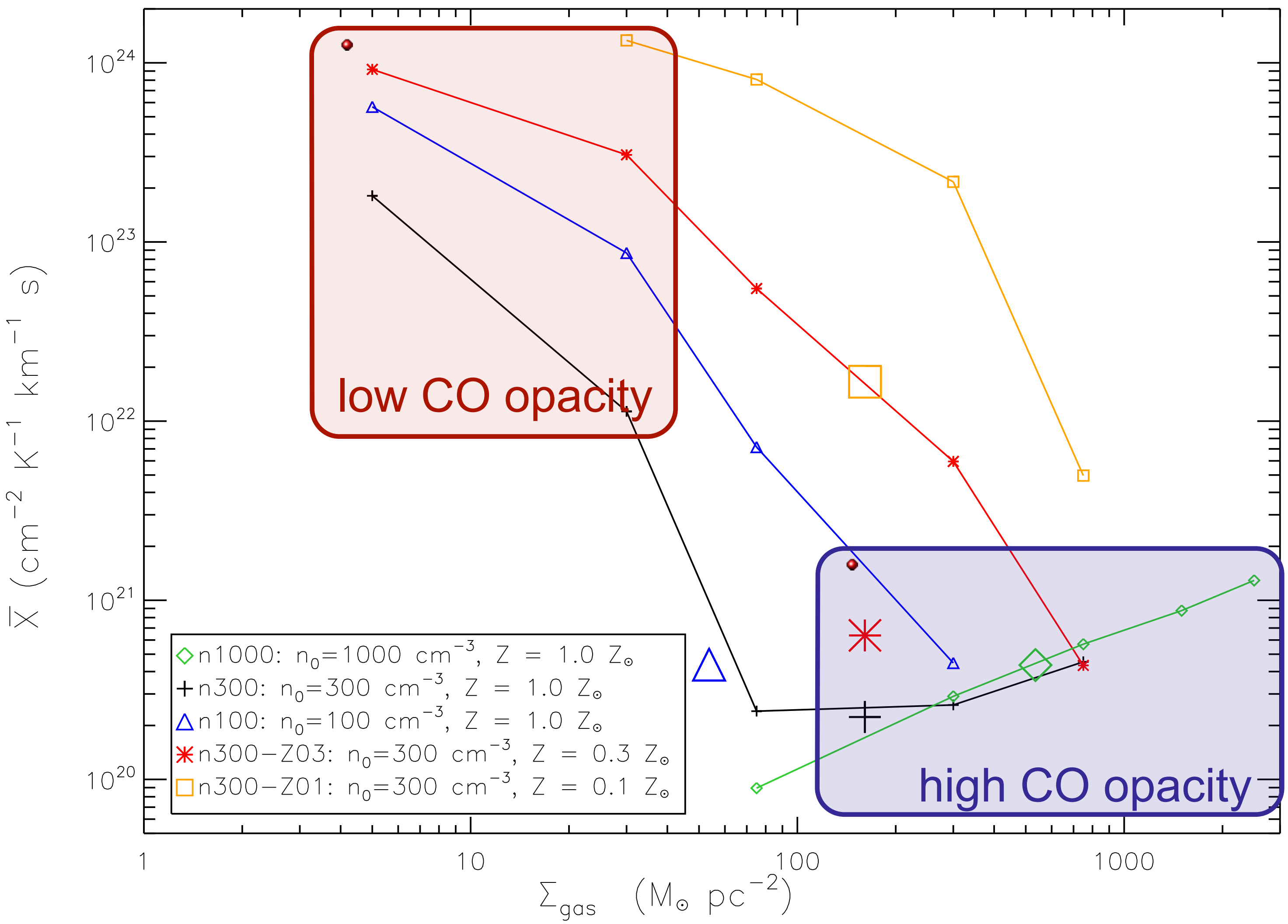
Figure 5. *X* factor for four models. N_{CO} is plotted as a function of $N_{\mathrm{H_2}}$. The colour of each point indicates the *X* factor. Inset figures show the colour scale and PDF of the *X* factor. The corresponding maps of $N_{\mathrm{H_2}}$, N_{CO} and the *X* factor from model n300-Z03 are shown in Fig. 4.

observed x-factor



Tacconi et al. (2008)

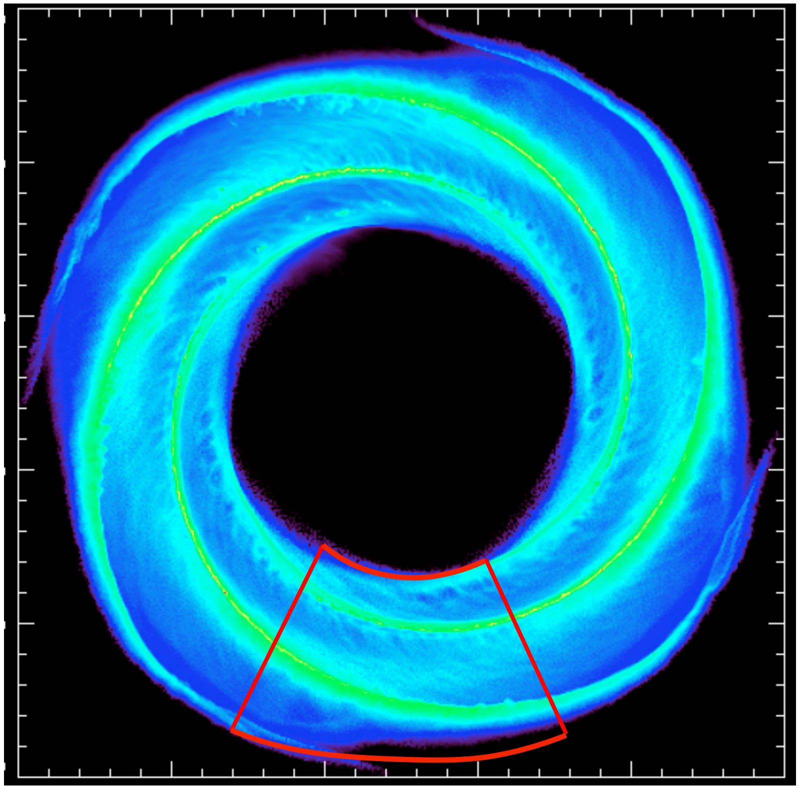
derived x-factor

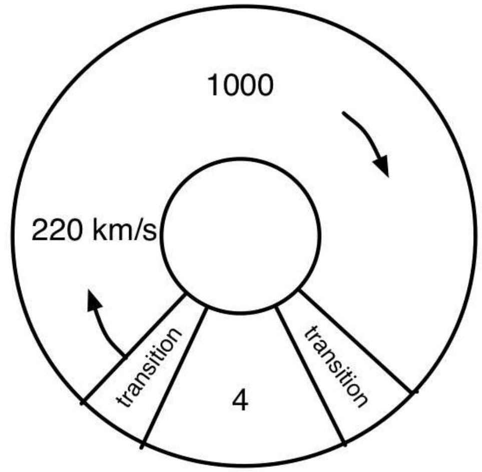


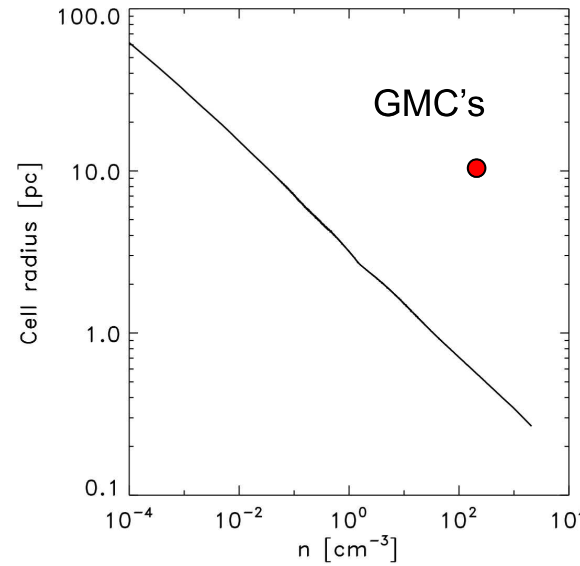
(Shetty, Glover, Dullemond, Klessen, MNRAS, 2011)

CO-dark gas

modeling molecular cloud formation



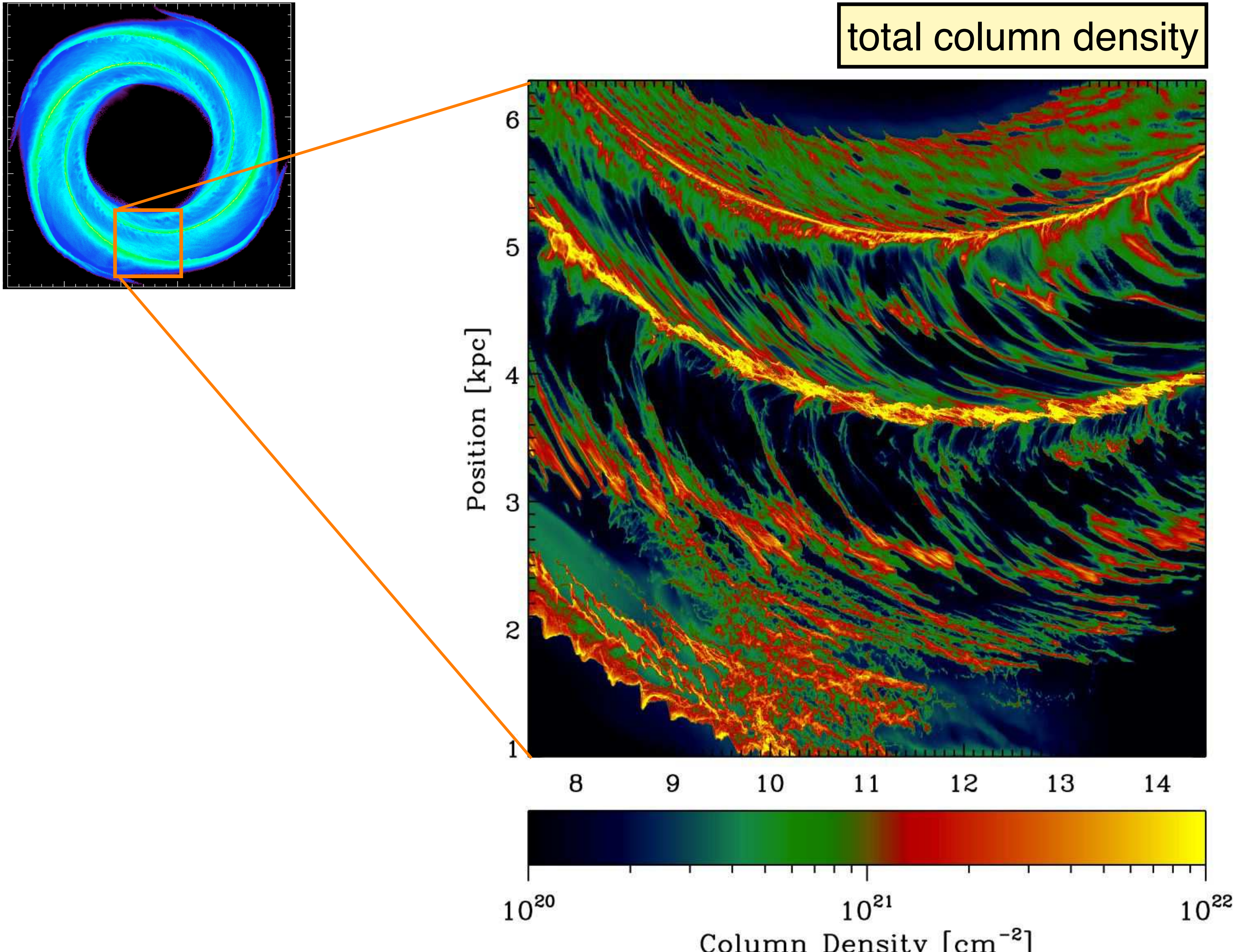




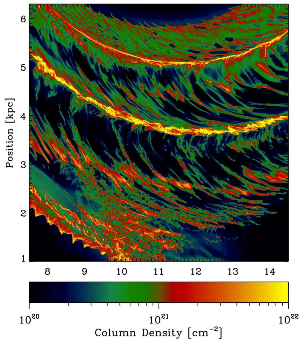
Simulation	Surface Density $M_\odot$ pc^{-2}	Radiation Field G_0
Milky Way	10	1
Low Density	4	1
Strong Field	10	10
Low & Weak	4	0.1

(Smith et al., 2014, MNRAS, 441, 1628)

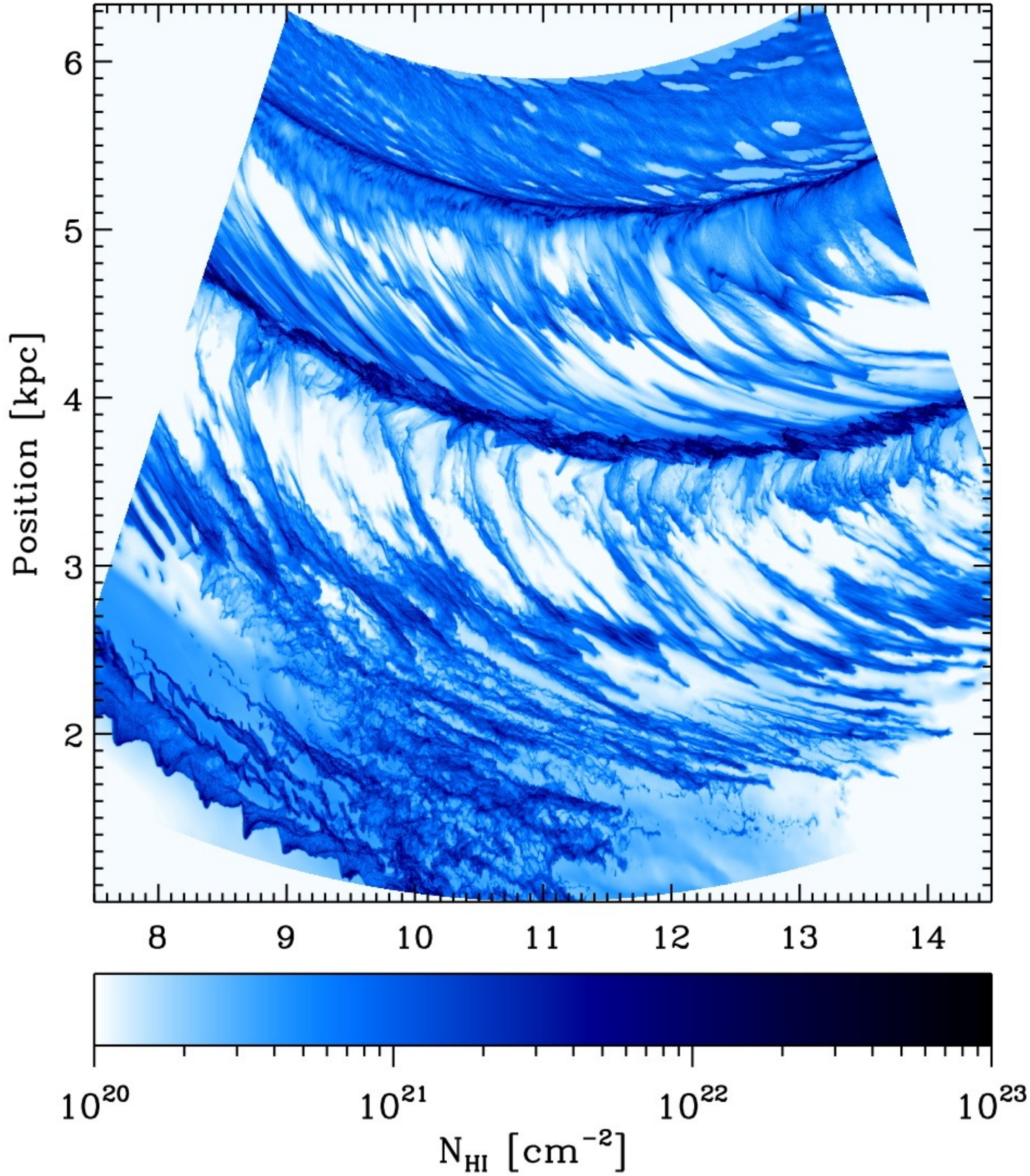
- Arepo moving mesh code *(Springel 2010)*
- time dependent chemistry *(Glover et al. 2007)* gives heating & cooling in a 2 phase medium
- two layers of refinement with mass resolution down to 4 $M_\odot$ in full Galaxy simulation
- UV field and cosmic rays
- TreeCol *(Clark et al. 2012)*
- external spiral potential *(Dobbs & Bonnell 2006)*
- no gas self-gravity, SN, or magnetic fields yet



(Smith et al., 2014, MNRAS, 441, 1628)

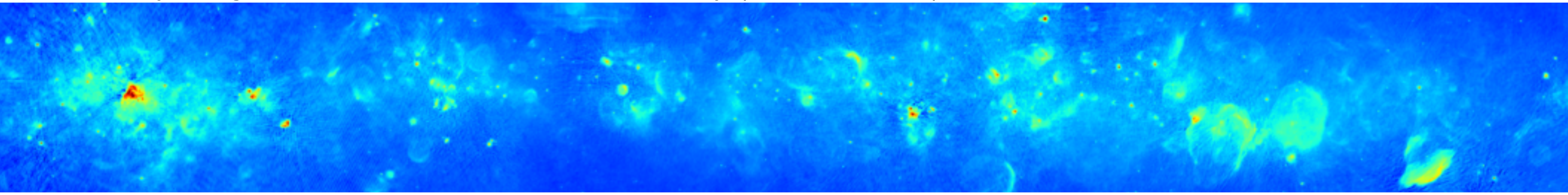


HI column density

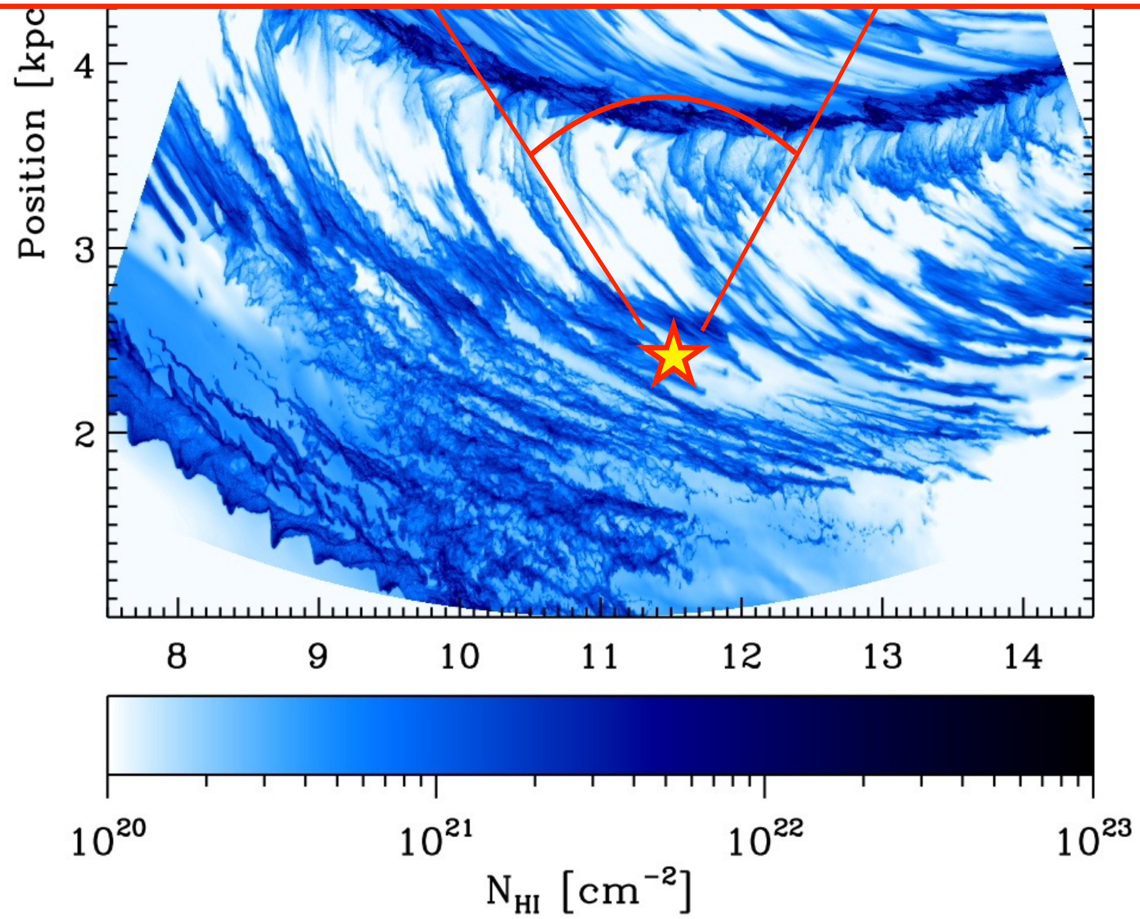


(Smith et al., 2014, MNRAS, 441, 1628)

preliminary image from THOR Galactic plane survey (PI H. Beuther): continuum emission around 21 cm



next step: produce all sky maps at various positions in the model galaxy (use RADMC-3D)



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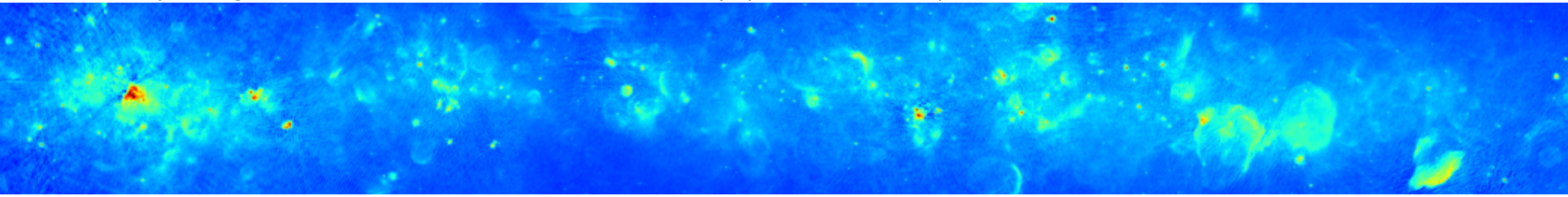

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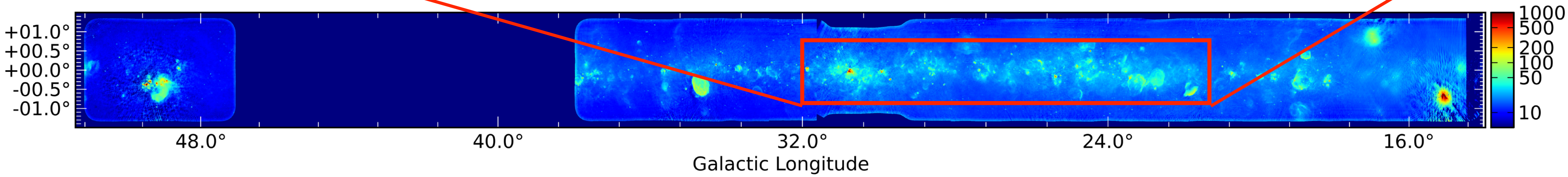
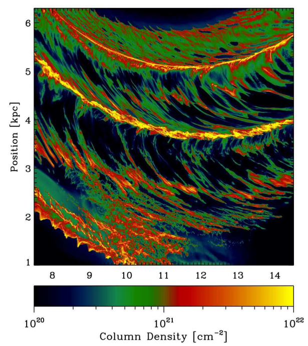
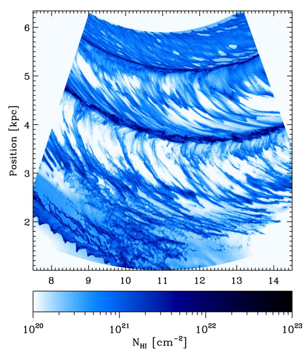
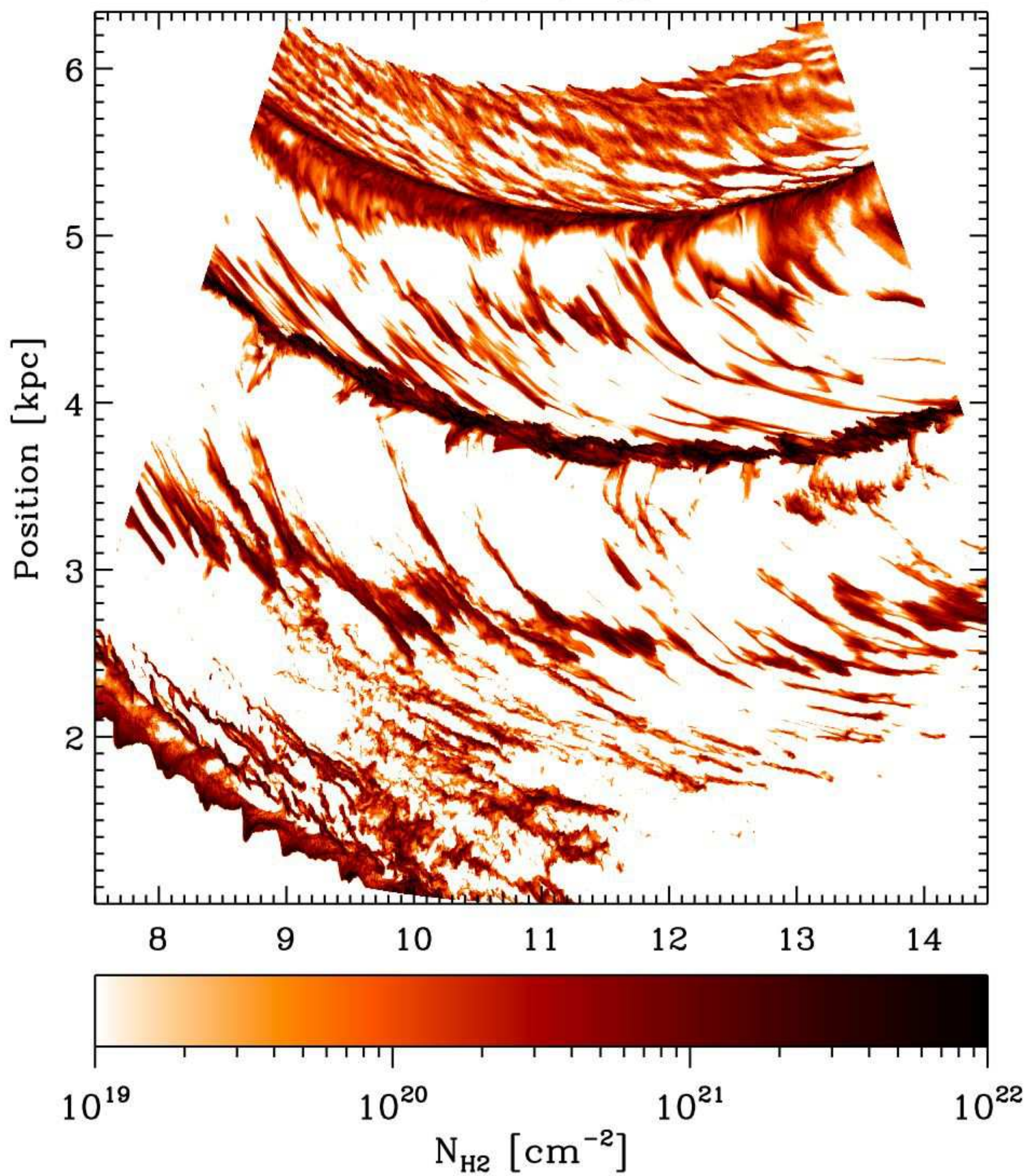


http://www.mpia.de/thor/Overview.html

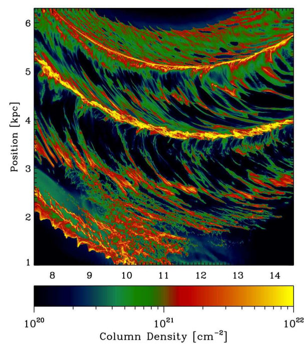


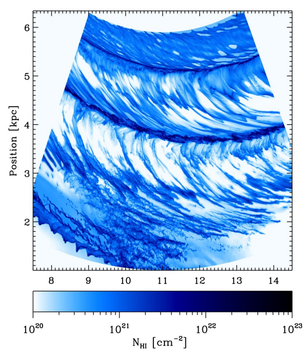


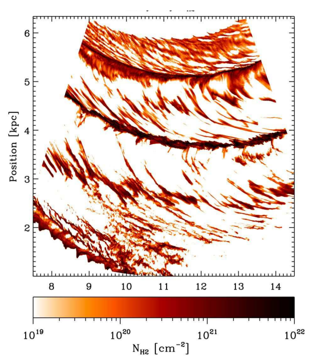
H_2 column density



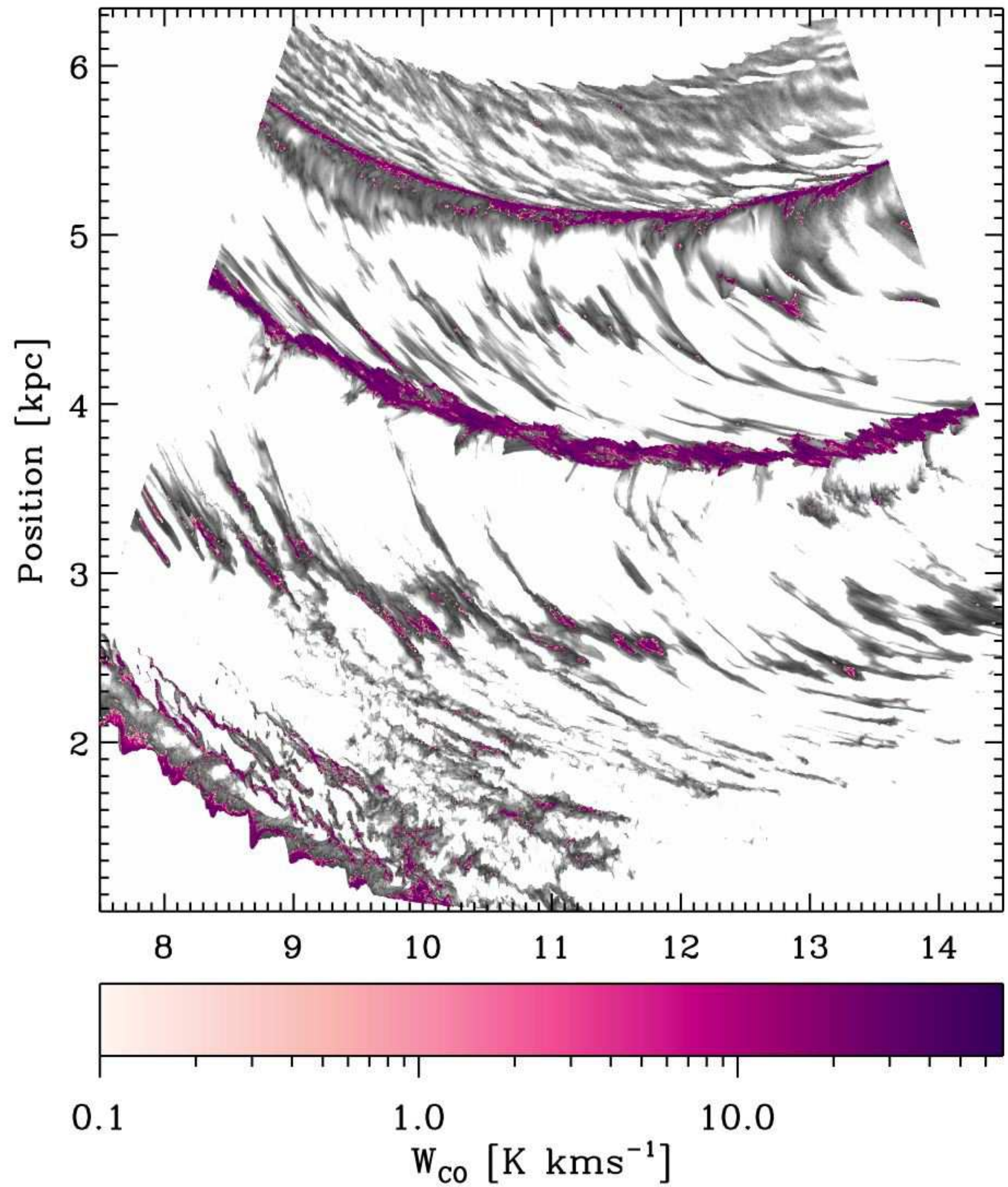
(Smith et al., 2014, MNRAS, 441, 1628)





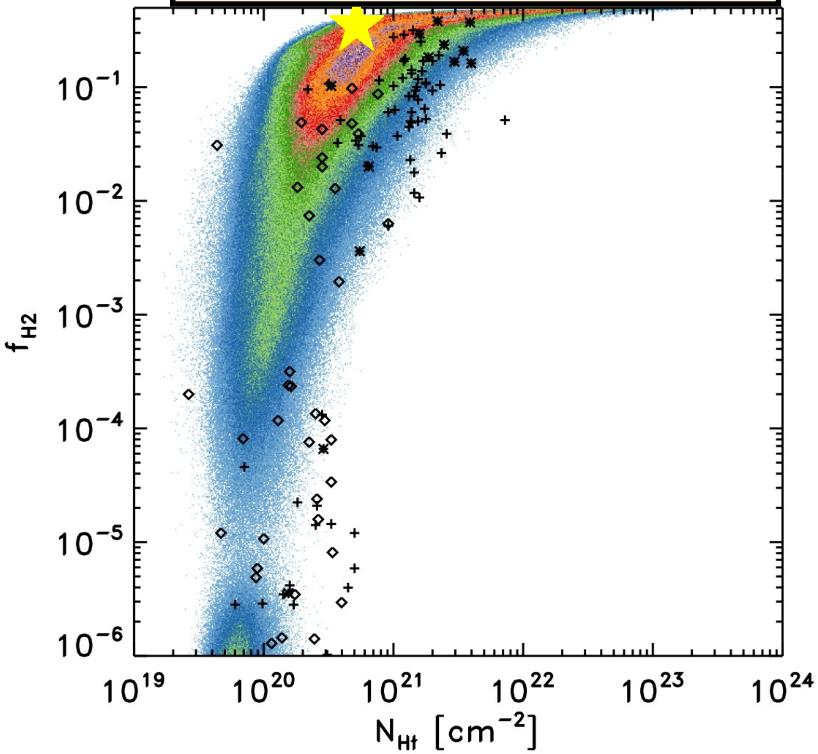


CO column density

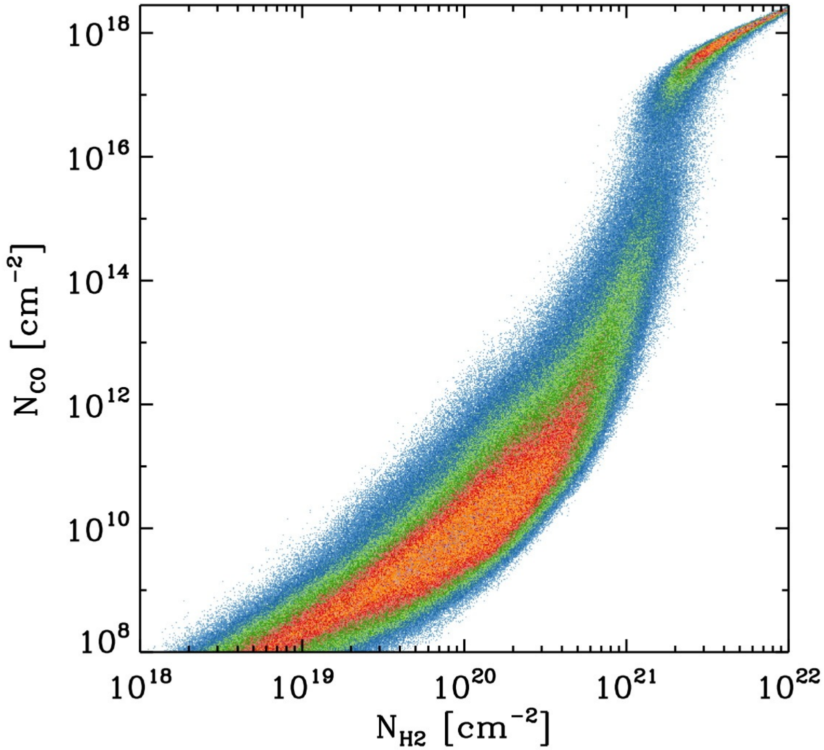


(Smith et al., 2014, MNRAS, 441, 1628)

H_2 fraction vs. column density N

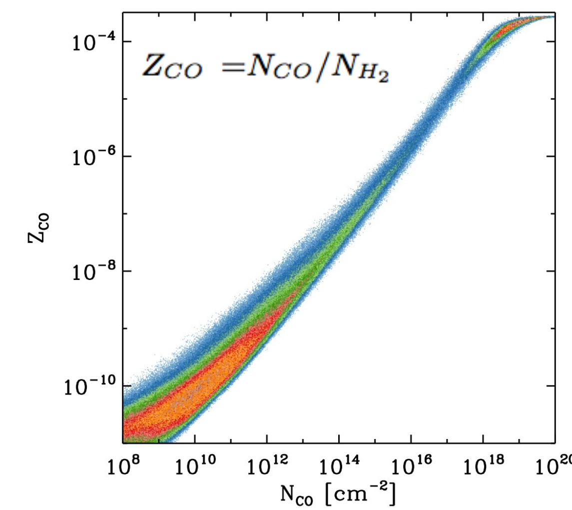


CO col. density vs. H_2 col. density



H_2 forms above column densities of 10^{20} cm^{-2}

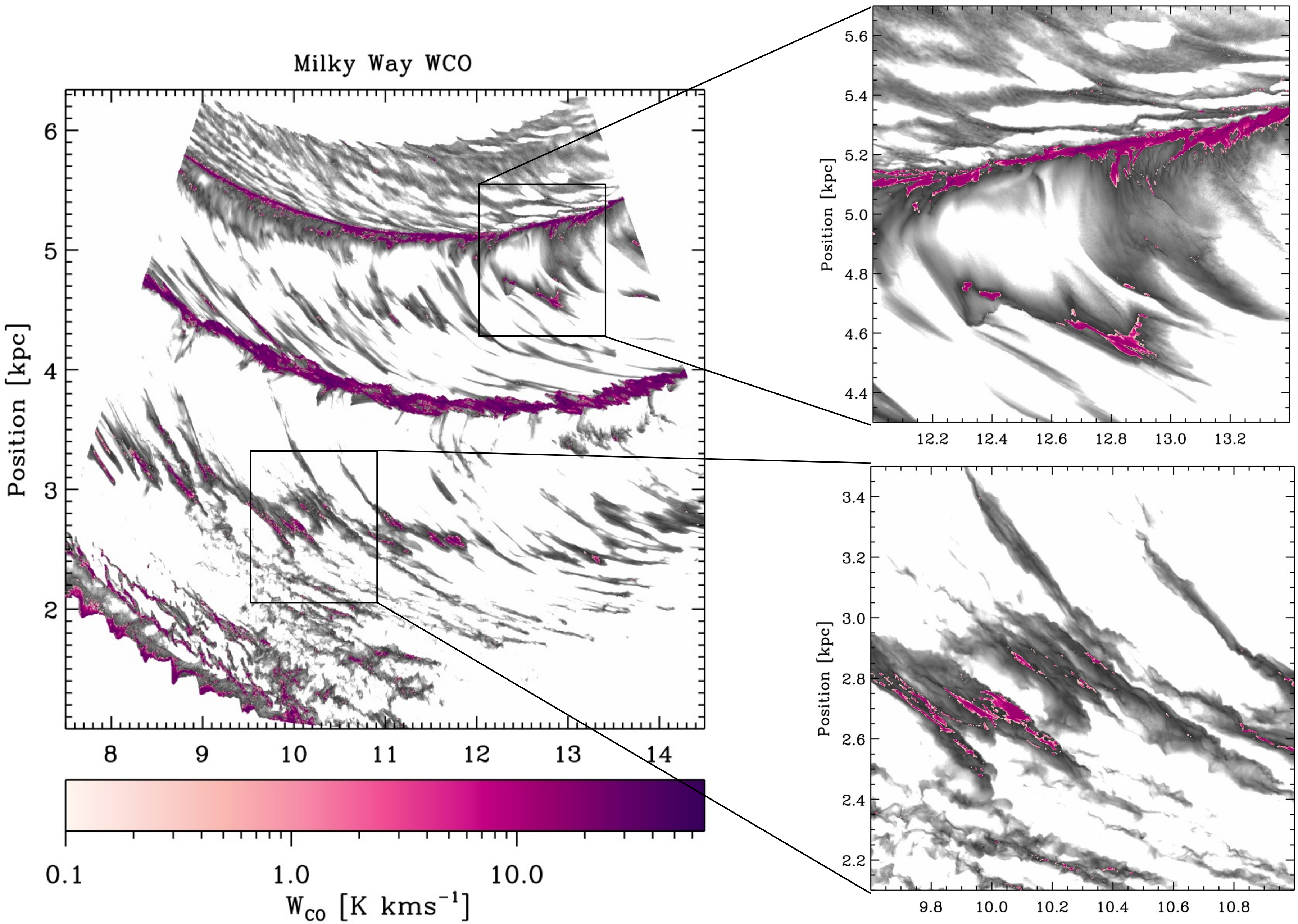
CO columns jump after $N_{H2} \sim 10^{21}$ cm^{-2}



$$log(Z_{CO}[cm^{-2}]) = -18.1 log(N_{CO}[cm^{-2}]) + 0.8.$$

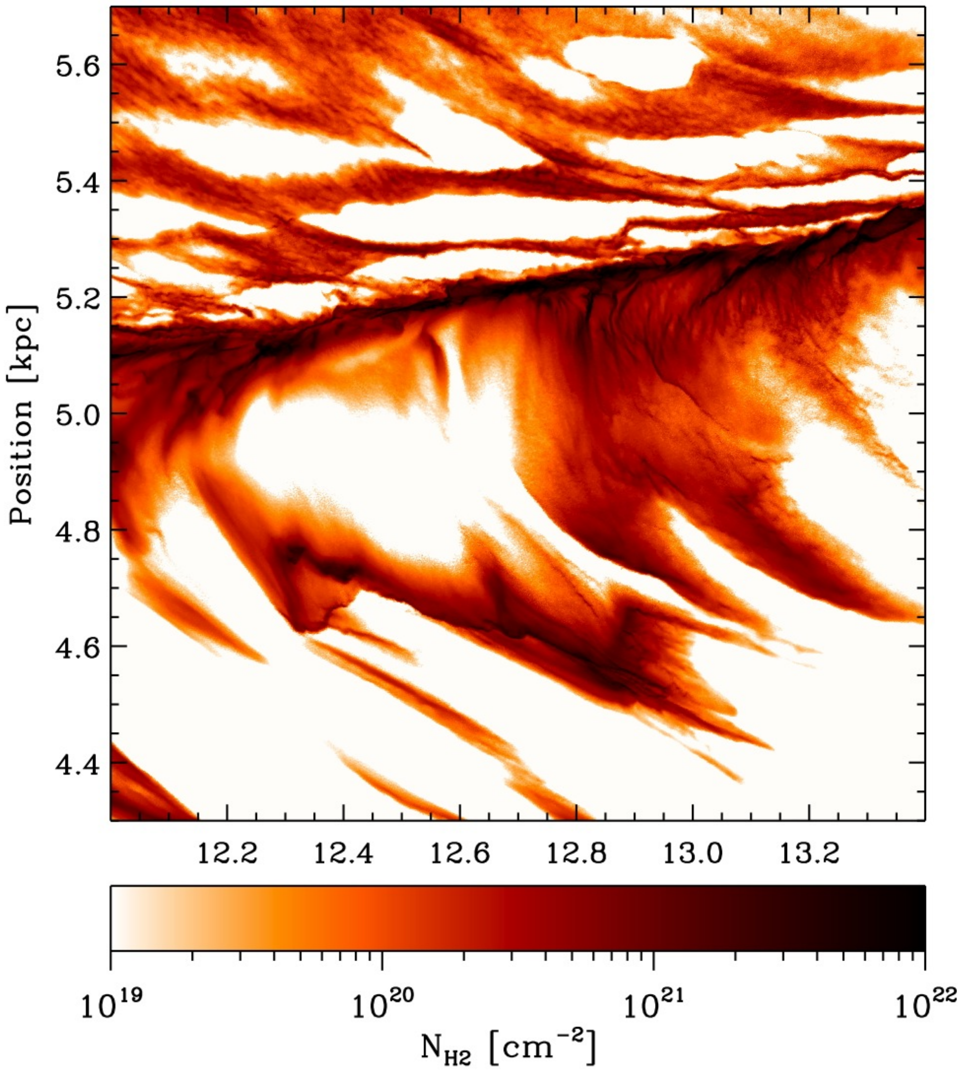
(Smith et al., 2014, MNRAS, 441, 1628)

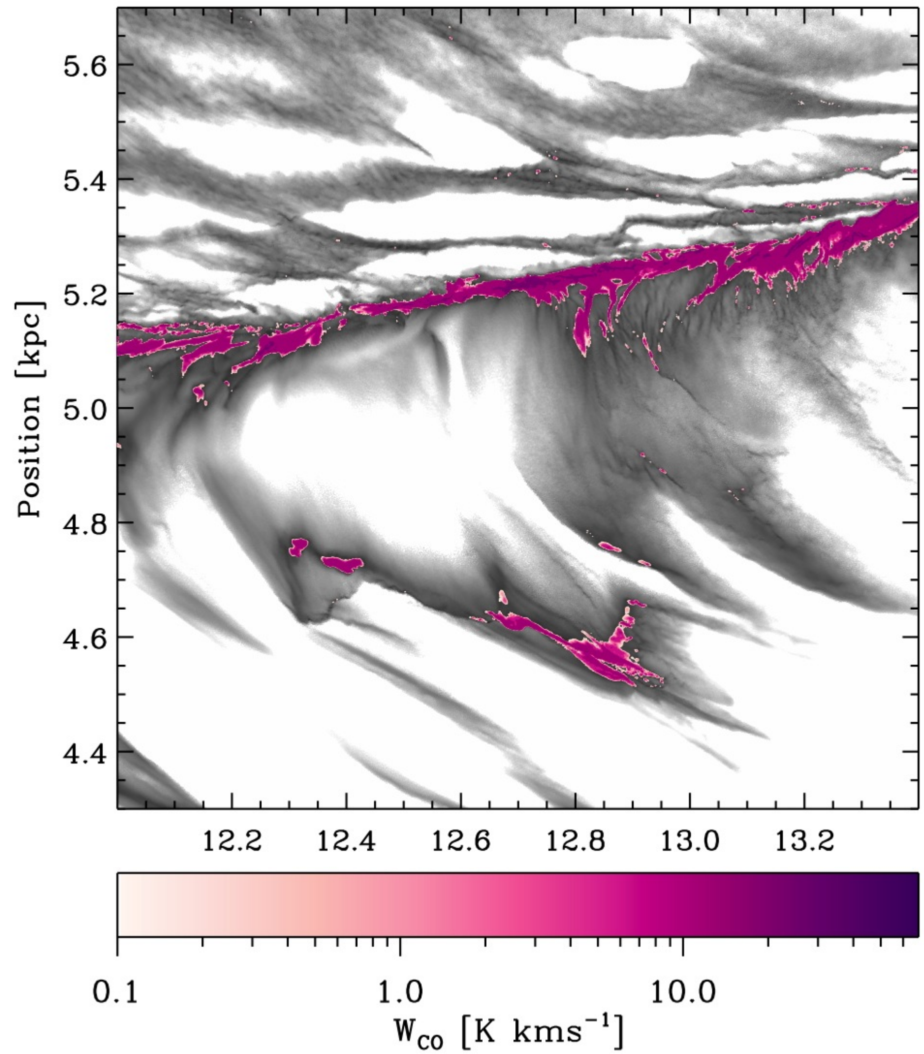
details of CO emission



(Smith et al., 2014, MNRAS, 441, 1628)

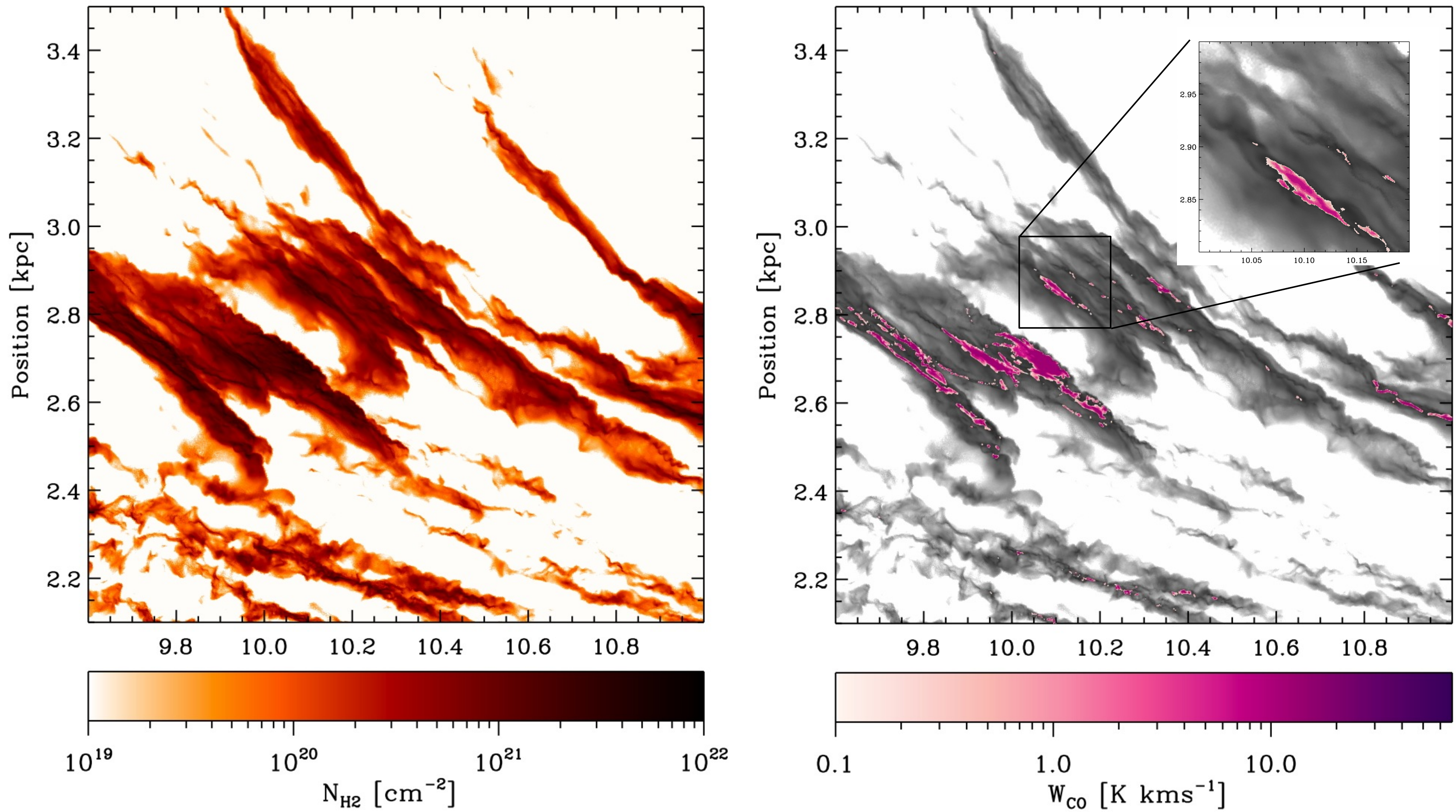
relation between CO and H_2





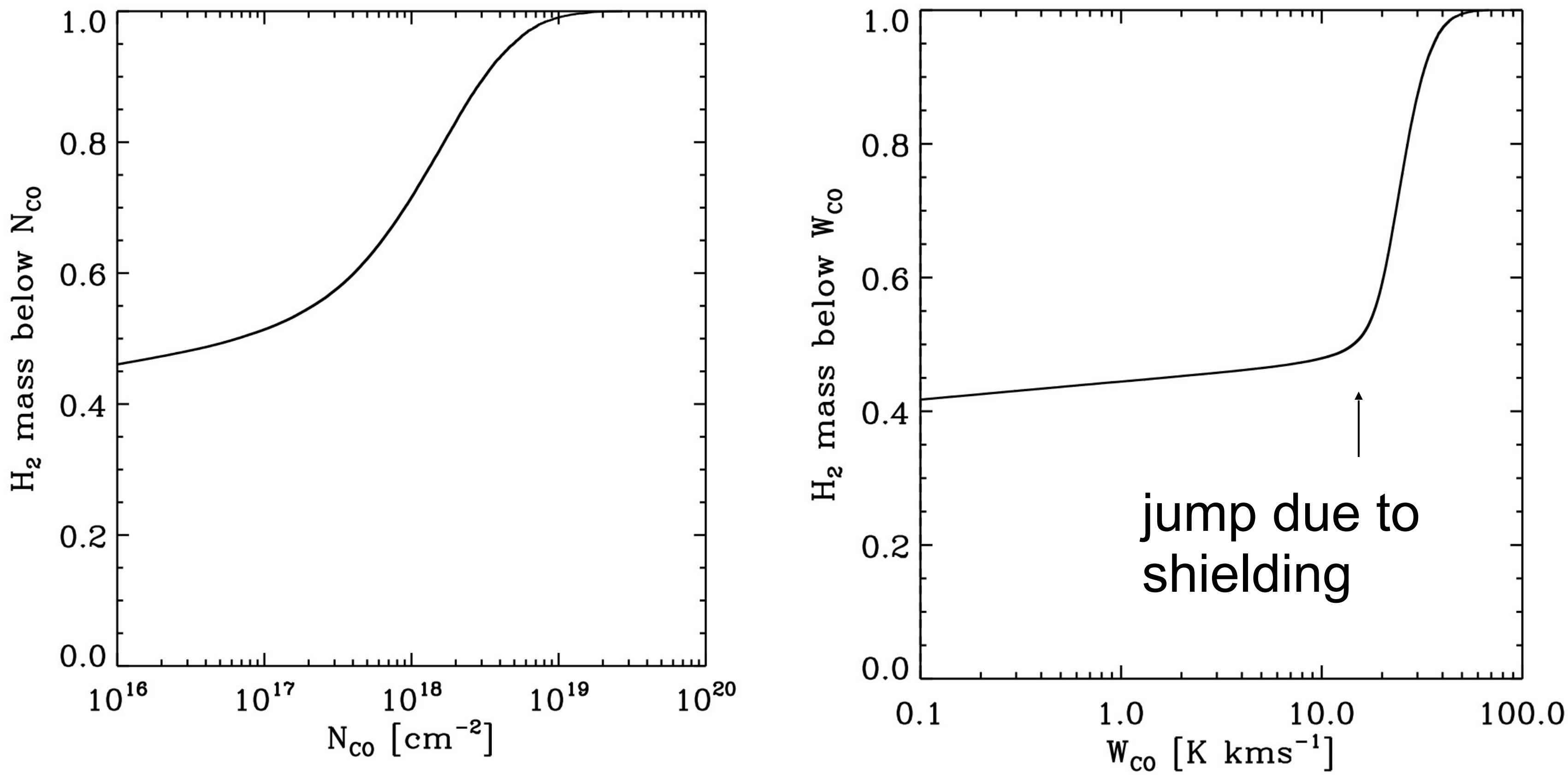
(Smith et al., 2014, MNRAS, 441, 1628)

relation between CO and H_2



Filamentary molecular clouds in inter-arm regions are likely only the observable parts of much larger structures.

dark gas fraction



46% molecular gas below CO column densities of 10^{16} cm^{-2}

42% has an integrated CO emission of less than 0.1 K kms^{-1}

$f_{DG} = 0.42$ $X_{co}=2.2 \times 10^{20}\ cm^{-2}K^{-1}km^{-1}s$

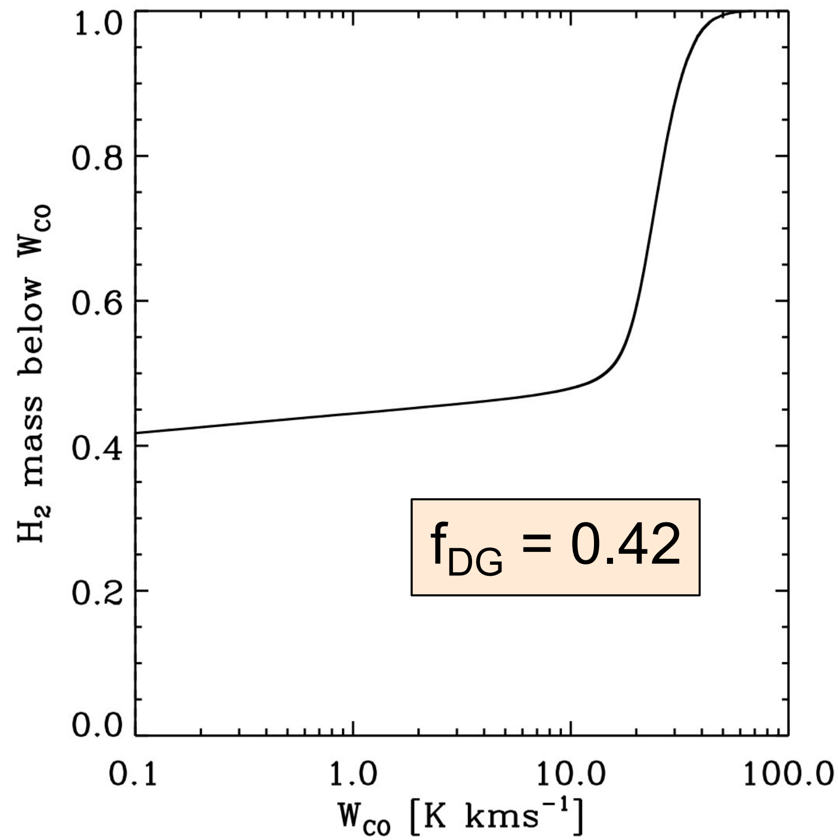
(Smith et al., 2014, MNRAS, 441, 1628)

dark gas fraction

Observational estimates:

Grenier et al. (2005)	f_{DG} = 0.33-0.5
Planck coll. (2011)*	f_{DG} = 0.54
Paradis et al. (2012)*	f_{DG} = 0.62
(inner f_{DG} = 0.71, outer f_{DG} = 0.43)	
Pineda et al. (2013)	f_{DG}= 0.3
Roman-Duval et al. (in prep.)	f_{DG} ~ 0.5

* dust methods have large uncertainties.



(Smith et al., 2014, MNRAS, 441, 1628)

is there CO-dark H_2 gas?

- there is increasing evidence, that a significant fraction of the H_2 gas in galaxies is not traced by CO (e.g. Pringle, Allen, Lubov 2001, Hosokawa & Inutsuka 2007, Clark et al. 2012)

- 3D simulations of colliding HI gas forming molecular clouds at the stagnation region performed by Paul Clark in Heidelberg

  - SPH (also with FLASH)
  - full fledged CO chemistry
  - TREECOL for calculating extinction
  - 'standard' dust model
  - sink particles to account for local collapse (star formation)
  - two models: slow and fast flow

further evidence form detailed colliding flow calculations

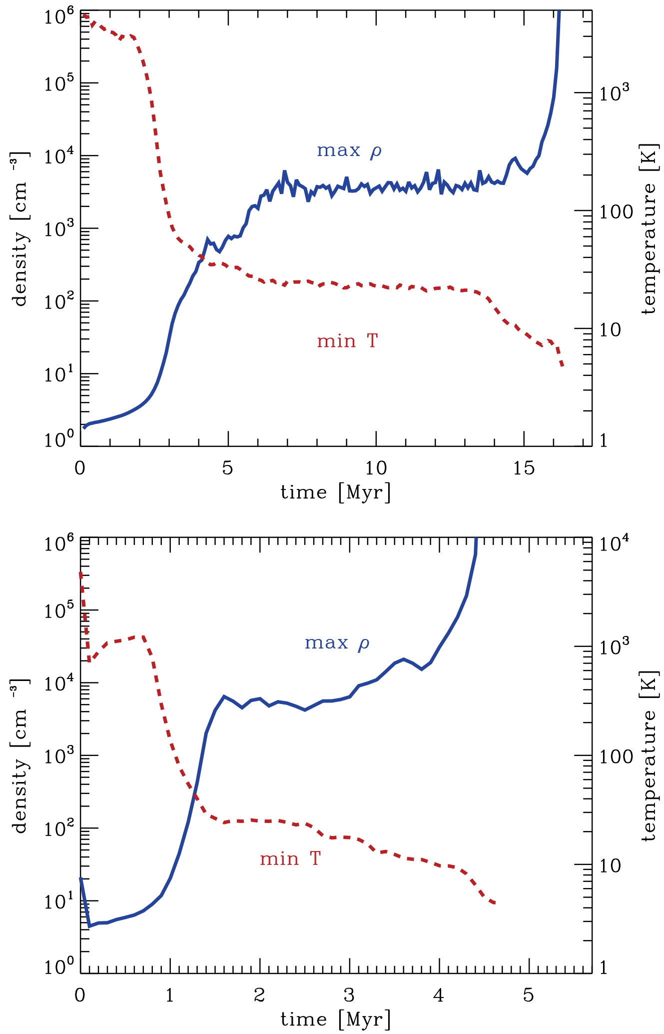
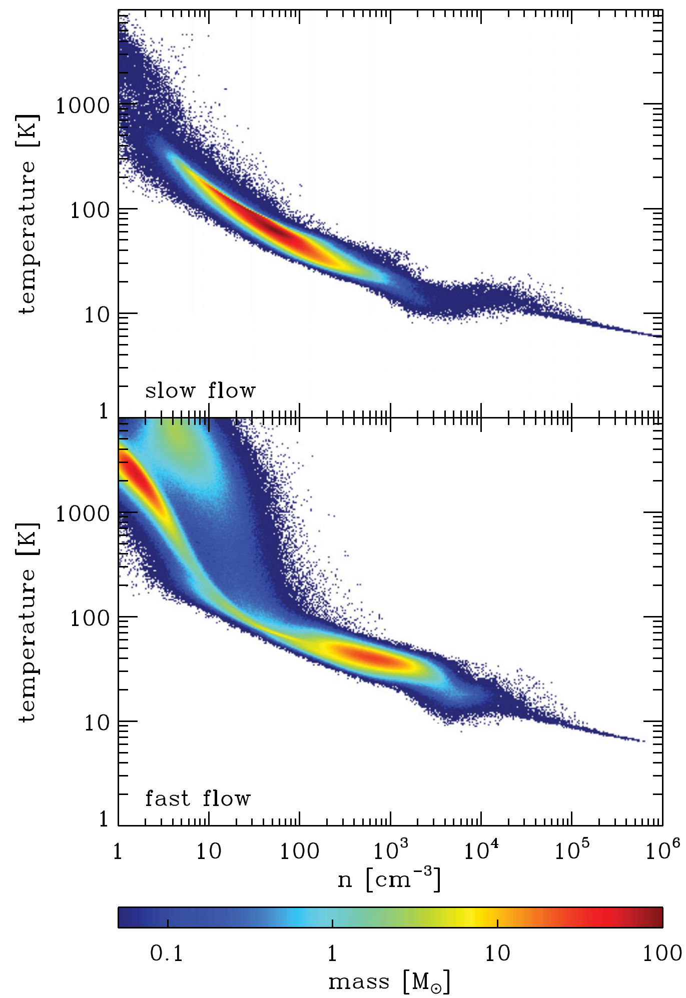


Figure 3. Evolution with time of the maximum density (blue, solid line) and minimum temperature (red, dashed line) in the slow flow (top panel) and the fast flow (bottom panel). Note that at any given instant, the coldest SPH particle is not necessarily the densest, and so the lines plotted are strictly independent of one another.



slow flow

fast flow

Figure 5. The gas temperature–density distribution in the flows at the onset of star formation.

Clark et al. (2012,MNRAS, 424, 2599)

see also Pringle, Allen, Lubov (2001), Hosokawa & Inutsuka (2007)

further evidence form detailed colliding flow calculations

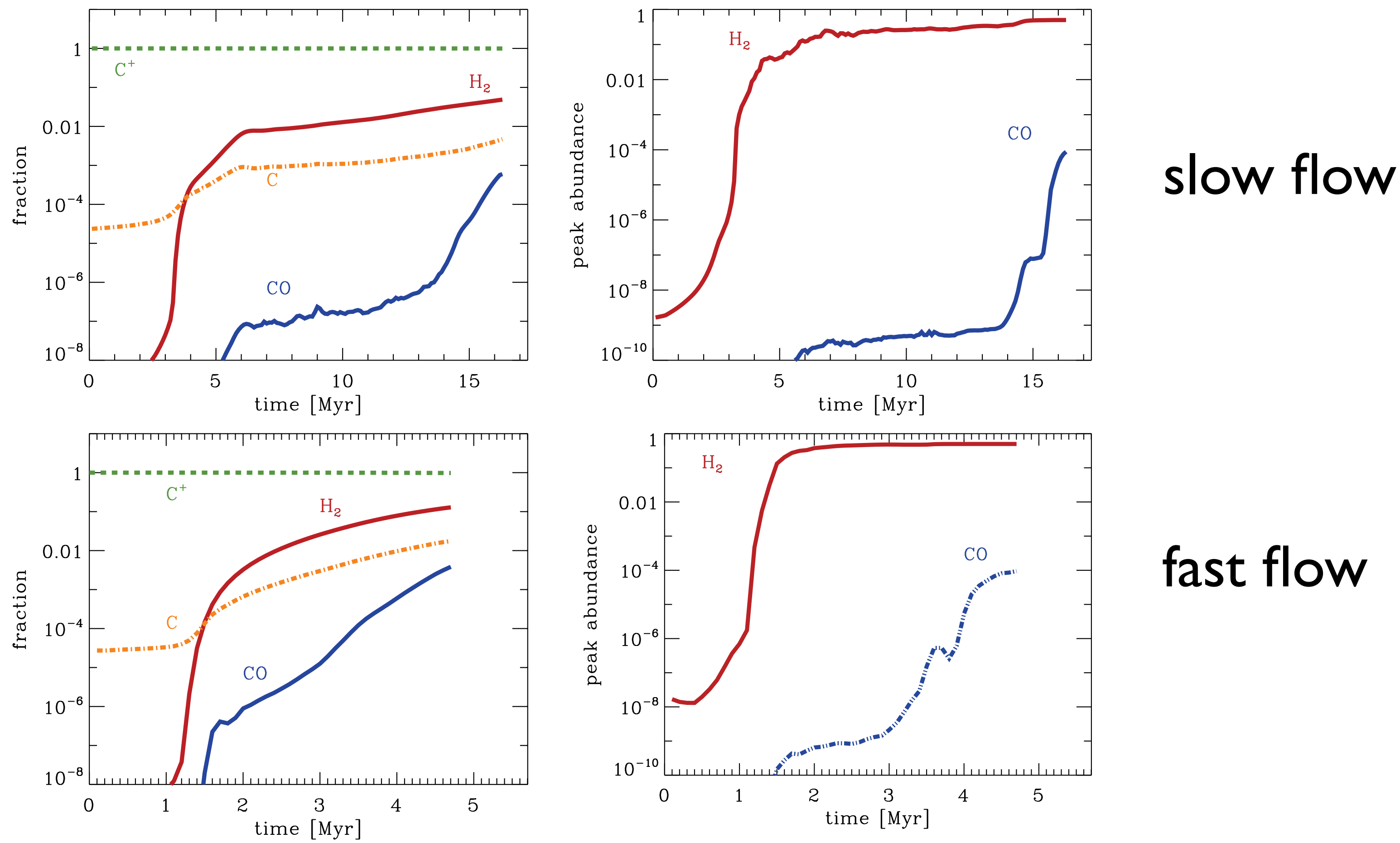
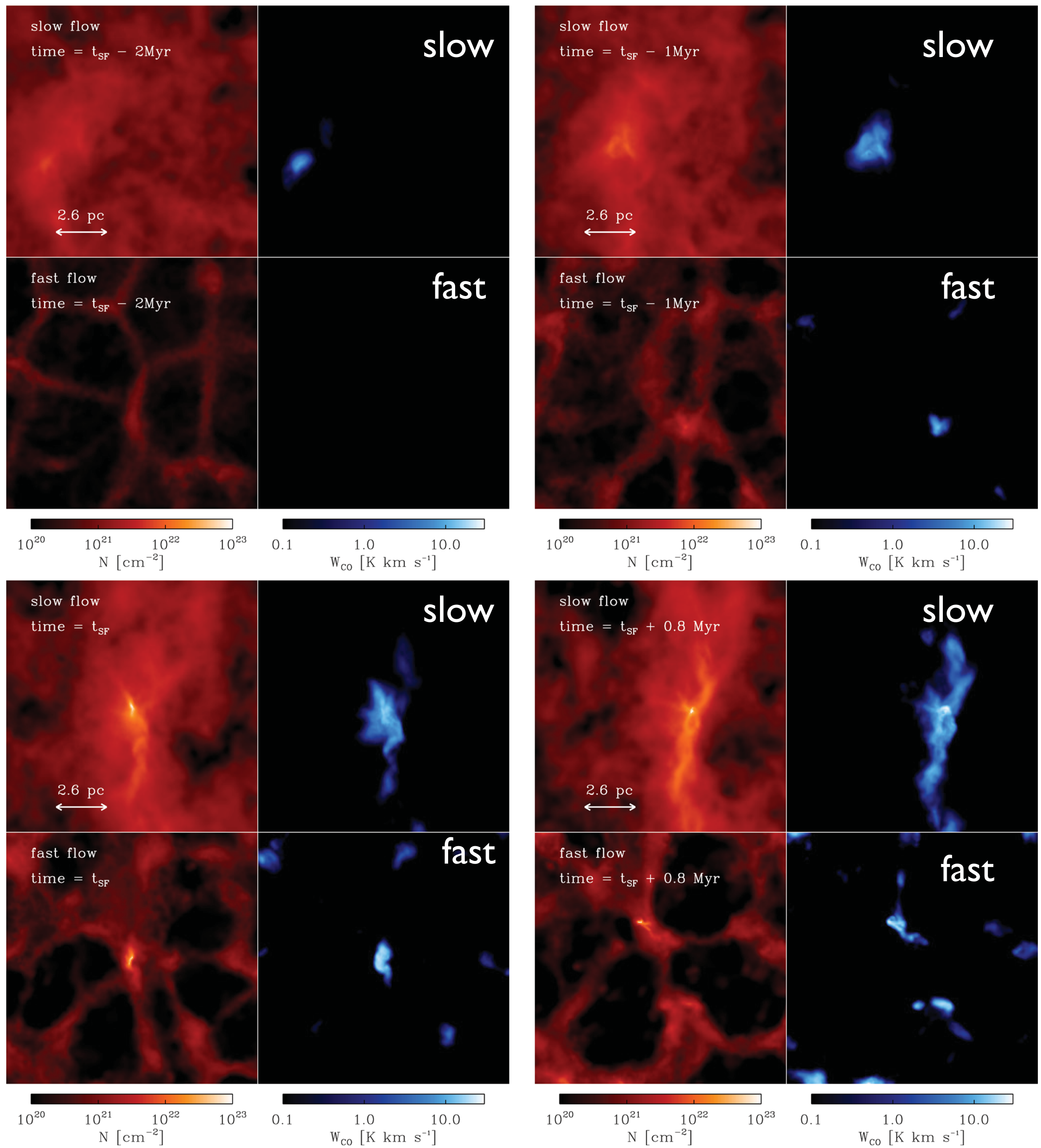


Figure 6. Chemical evolution of the gas in the flow. In the left-hand column, we show the time evolution of the fraction of the total mass of hydrogen that is in the form of H_2 (red solid line) for the 6.8 km s^{-1} flow (upper panel) and the 13.6 km s^{-1} flow (lower panel). We also show the time evolution of the fraction of the total mass of carbon that is in the form of C^+ (green dashed line), C (orange dot–dashed line) and CO (blue double-dot–dashed line). In the right-hand column, we show the peak values of the fractional abundances of H_2 and CO. These are computed relative to the total number of hydrogen nuclei, and so the maximum fractional abundances of H_2 and CO are 0.5 and 1.4×10^{-4}, respectively. Again, we show results for the 6.8 km s^{-1} flow in the upper panel and the 13.6 km s^{-1} flow in the lower panel. Note that the scale of the horizontal axis differs between the upper and lower panels.

Clark et al. (2012,MNRAS, 424, 2599)

see also Pringle, Allen, Lubov (2001), Hosokawa & Inutsuka (2007)



H_2 column

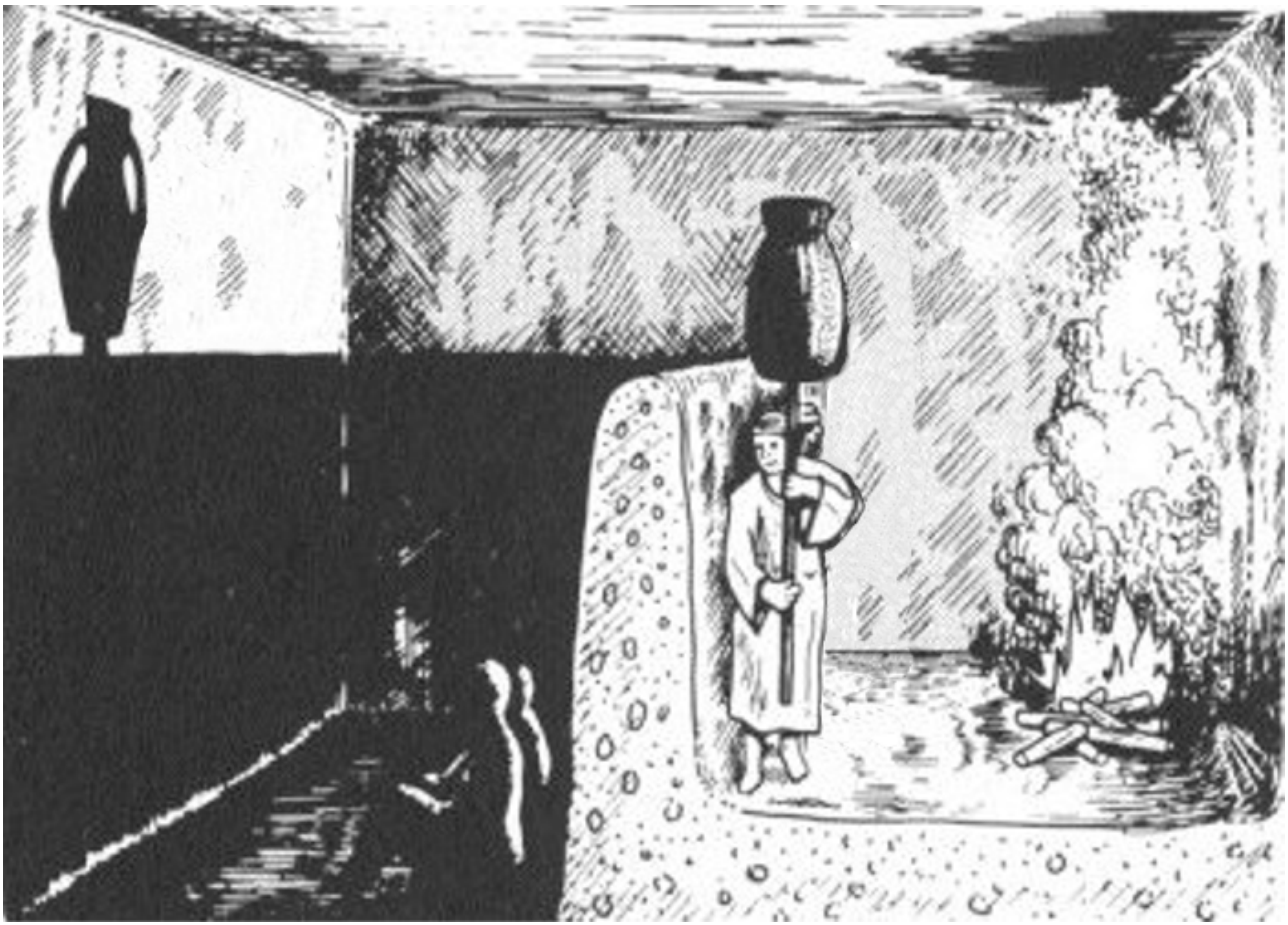
CO emission

fraction of CO dark gas will also change with metallicity and with ambient radiation field

Clark et al. (2012,MNRAS, 424, 2599)

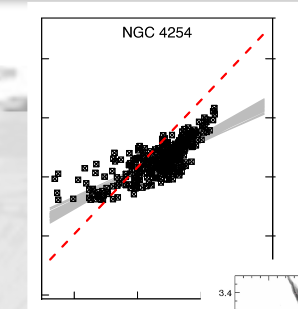
Summary

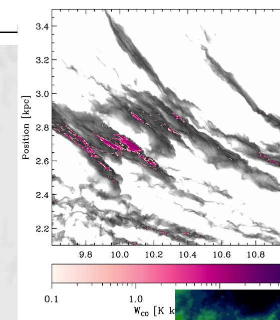
Star formation is intrinsically a multi-scale and multi-physics problem. Many different processes need to be considered simultaneously.

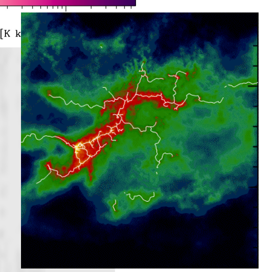


* The Republic (514a-520a)

Star formation is intrinsically a multi-scale and multi-physics problem. Many different processes need to be considered simultaneously.







- hierarchical Bayesian statistics indicated galaxy to galaxy variations in the KS relation with typically sublinear slope
  → *how much diffuse CO gas is there*
- detailed (M)HD calculations with time-dependent chemistry allow us to study the properties of CO-dark H2 gas
  → *implications for interpreting observational data?*
- molecular clouds are filamentary, but filament parameters (width, slope, central density) may vary significantly
  → *what does it mean for star cluster formation?*
- next steps:
  multi-physics simulations with Arepo and FLASH for comparison with existing survey data

* The Republic (514a-520a)

Laszlo Szücs, image from criticalthinking-mc205.wikispaces.com thanks