

PART III

ISM: Gas In Galaxies

1. Galaxy Formation Lite

- The main physics of galaxy formation is captured by Mo, Mao & White model*.
- Cooling of gas in the halo (or inflow along cool flows) delivers cool gas at the bottom of the potential well (=halo center).
- The gas settles into a *galactic disk*.

* Mon. Not. R. Astron. Soc. **295**, 319–336 (1998)

Galactic Disk

Quiz:

? *Why does cooling gas settle into a disk?*

- A. Galaxies are observed to have disks.
- B. Angular momentum is conserved.
- C. The gravity of dark matter compresses gas into a disk.
- D. The pressure of hot halo compresses gas into a disk.
- E. Gas flows along circular orbits.

Galactic Disk

- Mass of a disk is a given fraction of the halo mass ($\sim 5\%$).

$$M_d = m_d M_h$$

- Disk has an exponential surface density profile.

$$\Sigma(R) = \Sigma_0 \exp(-R/R_d)$$

$$M_d = 2\pi \Sigma_0 R_d^2$$

- Angular momentum of the disk is a given fraction of the halo angular momentum.

$$J_d = 4\pi \Sigma_0 R_d^3 V_c$$

$$J_d = j_d J_h$$

Galactic Disk

- Halo angular momentum is well understood:

$$\lambda = \frac{J_h |E_h|^{1/2}}{GM_h^{5/2}}$$

- Spin parameter λ is lognormally-distributed

$$p(\lambda)d\lambda = \frac{1}{\sqrt{2\pi}\sigma_\lambda} \exp\left[-\frac{\ln^2(\lambda/\bar{\lambda})}{2\sigma_\lambda^2}\right] \frac{d\lambda}{\lambda}$$

- with $\bar{\lambda} = 0.05$ and $\sigma_\lambda = 0.5$.

Galactic Disk

- The last step – a connection between the halo mass and the disk circular velocity:

$$V_c \propto V_{\text{vir}} = \left(\frac{GM_h}{r_{\text{vir}}} \right)^{1/2}$$

- MMW98 model assumes the coefficient of proportionality is 1, but it does not have to be.

Galactic Disk

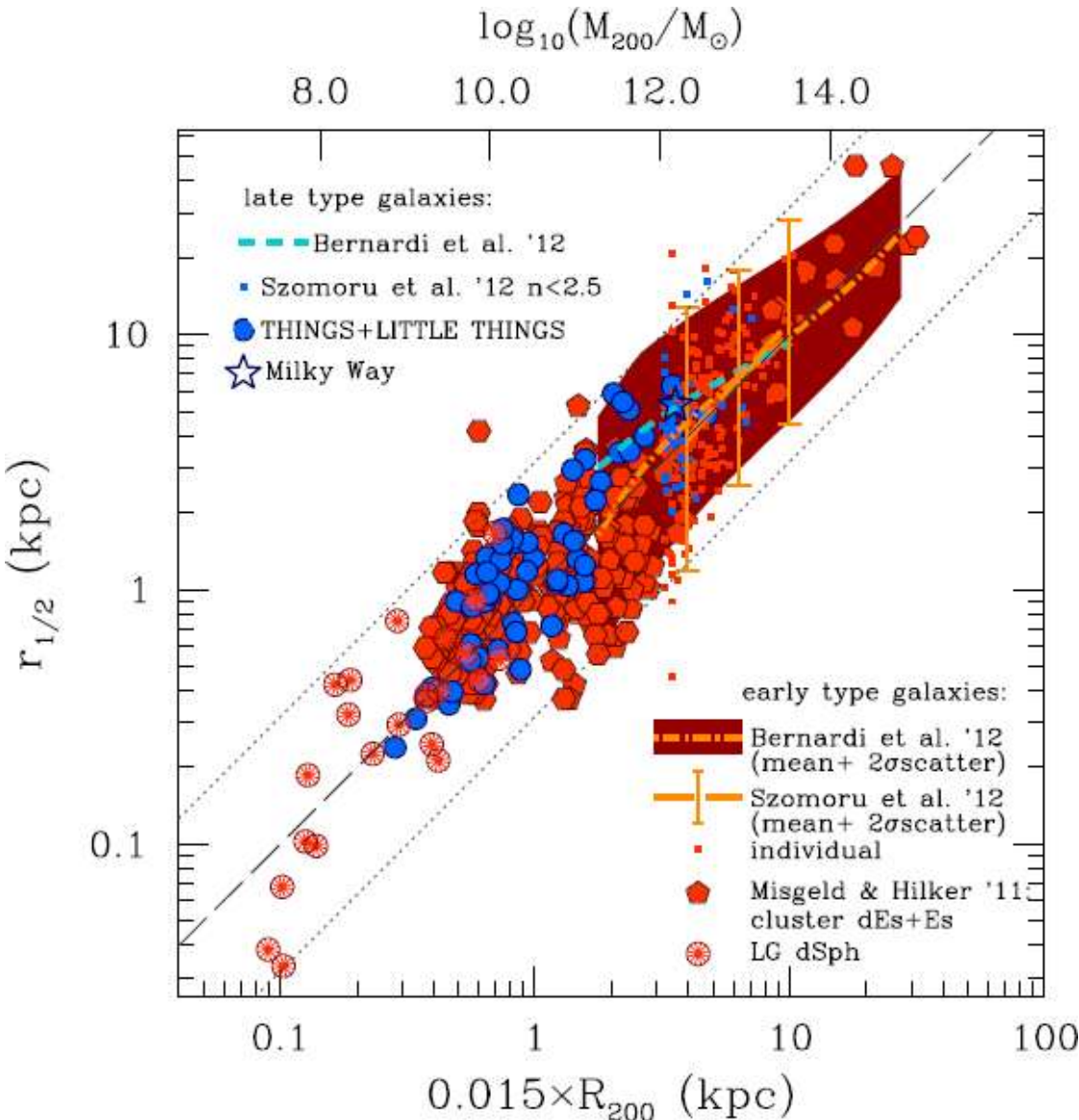
- NFW profile:

$$\left(\frac{V_c(r)}{V_{\text{vir}}}\right)^2 = \frac{1}{x} \frac{\ln(1+cx) - cx/(1+cx)}{\ln(1+c) - c/(1+c)}, \quad x = \frac{r}{r_{\text{vir}}}$$

- V_c is maximized at $cx = 2.16$.
 - $V_{\text{max}} = 1.0V_{\text{vir}}$ for $c = 3$;
 - $V_{\text{max}} = 1.2V_{\text{vir}}$ for $c = 10$;
 - $V_{\text{max}} = 1.6V_{\text{vir}}$ for $c = 30$;

$$V_{\text{vir}} = 163 \text{ km/s} \left(\frac{M_h}{10^{12} M_{\odot}}\right)^{1/3} \left(\frac{H(a)}{H_0}\right)^{1/3}$$

Disk – Halo Connection



- Sizes of disks are directly proportional to the sizes of their dark matter halos (a-la MMW98)
- Observed scatter = scatter in λ

$$p(\lambda)d\lambda = \frac{1}{\sqrt{2\pi}\sigma_{\lambda}} \exp\left[-\frac{\ln^2(\lambda/\bar{\lambda})}{2\sigma_{\lambda}^2}\right] \frac{d\lambda}{\lambda}$$

2. Galactic Disks

- Surface density of the disk $\Sigma(R)$ (M_{\odot}/pc^2).
- Circular velocity of the disk

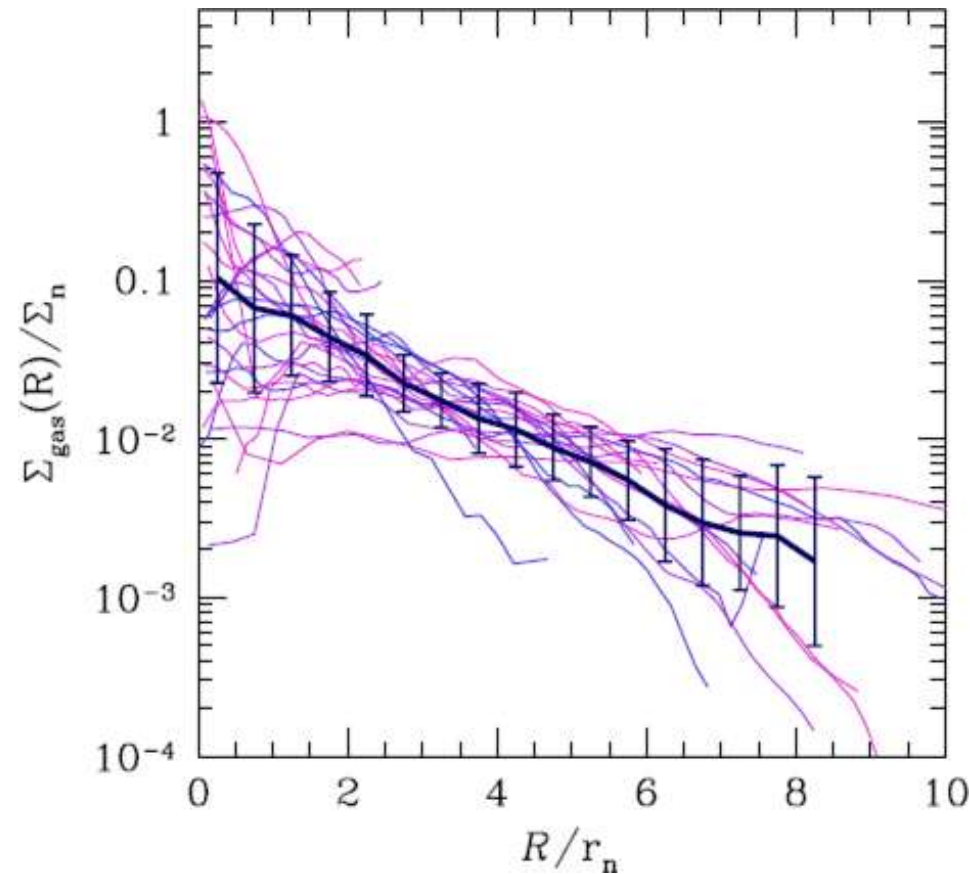
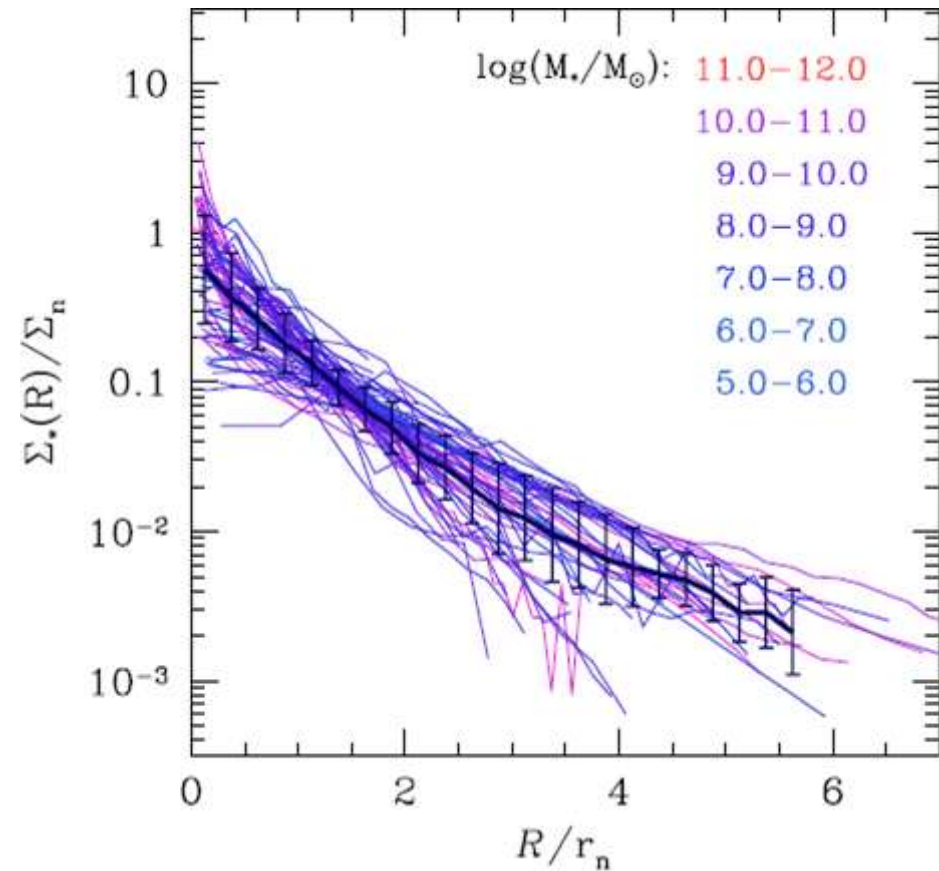
$$V_c^2(R) = -R \int_0^{\infty} S(k) J_1(kR) k dk$$

$$S(k) = -2\pi G \int_0^{\infty} J_0(kR) \Sigma(R) R dR$$

- In a vertical (usually z-) direction the disk profile is described by a “scale height” h .
- Different components have different scale heights.

Density Profile

- Both stellar and gaseous disks are \sim exponential, but gaseous disks are larger.



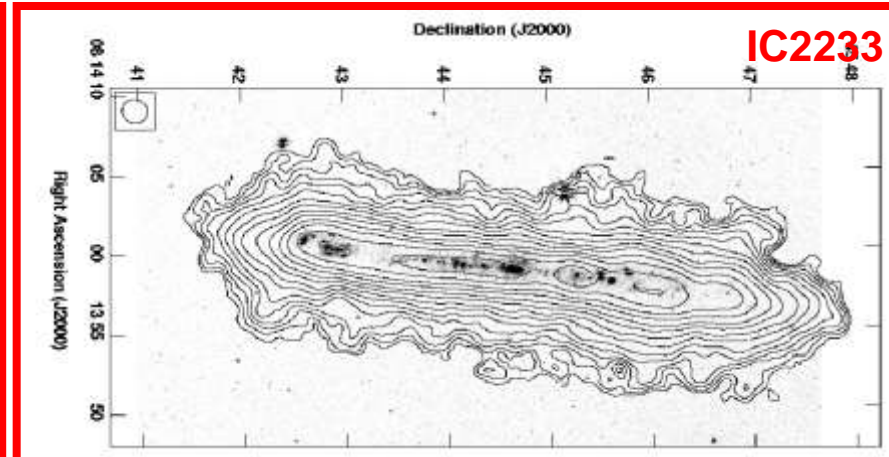
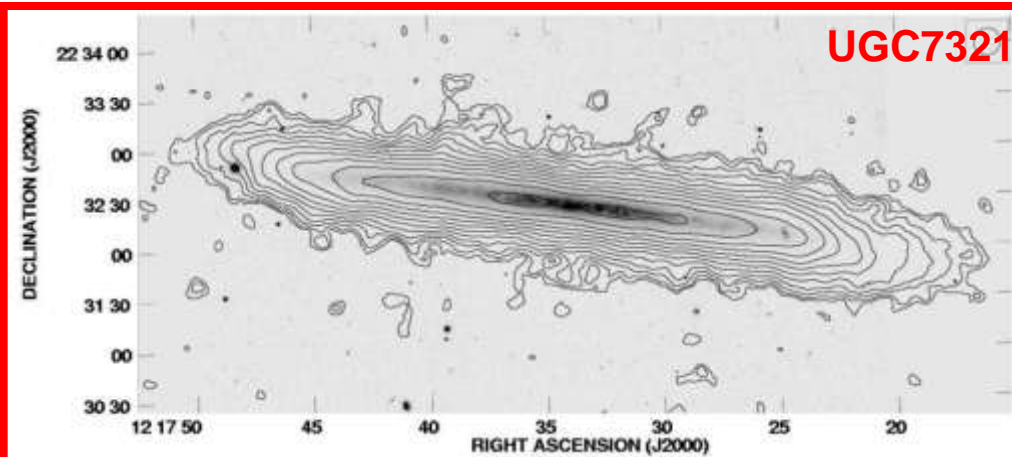
Scale Heights

Galaxy Mass

Stellar height

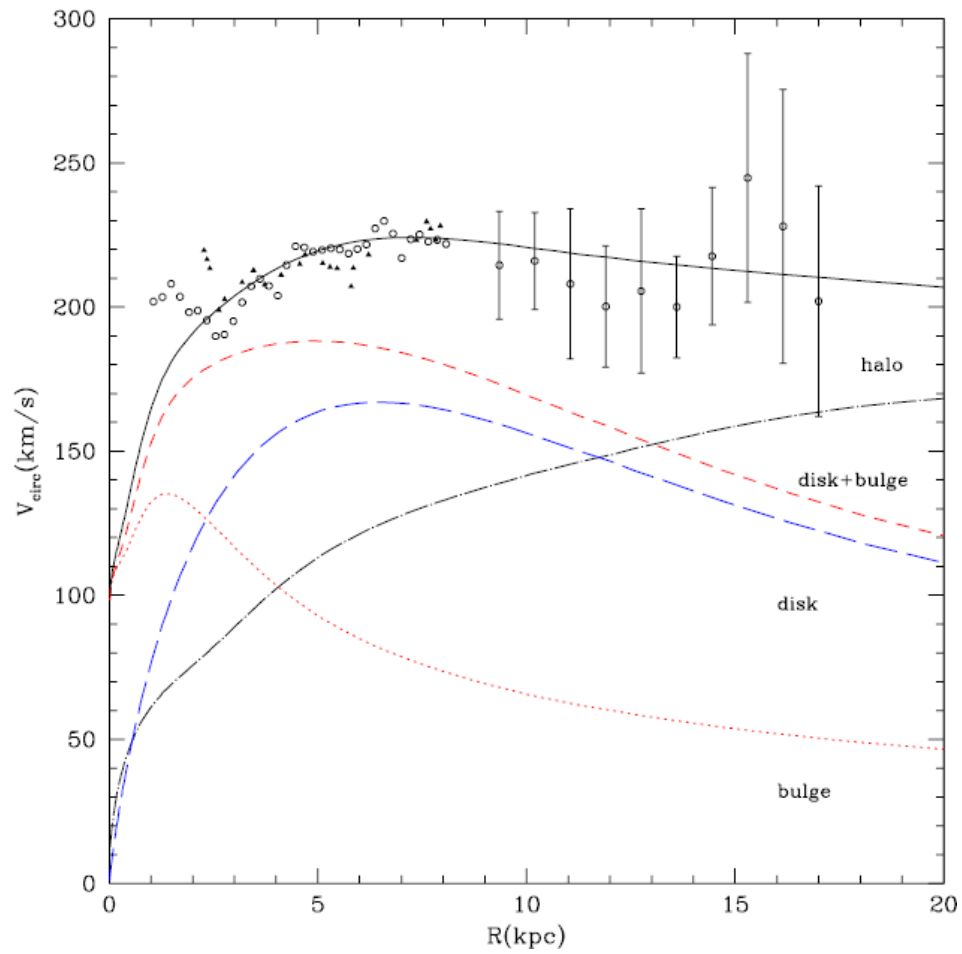
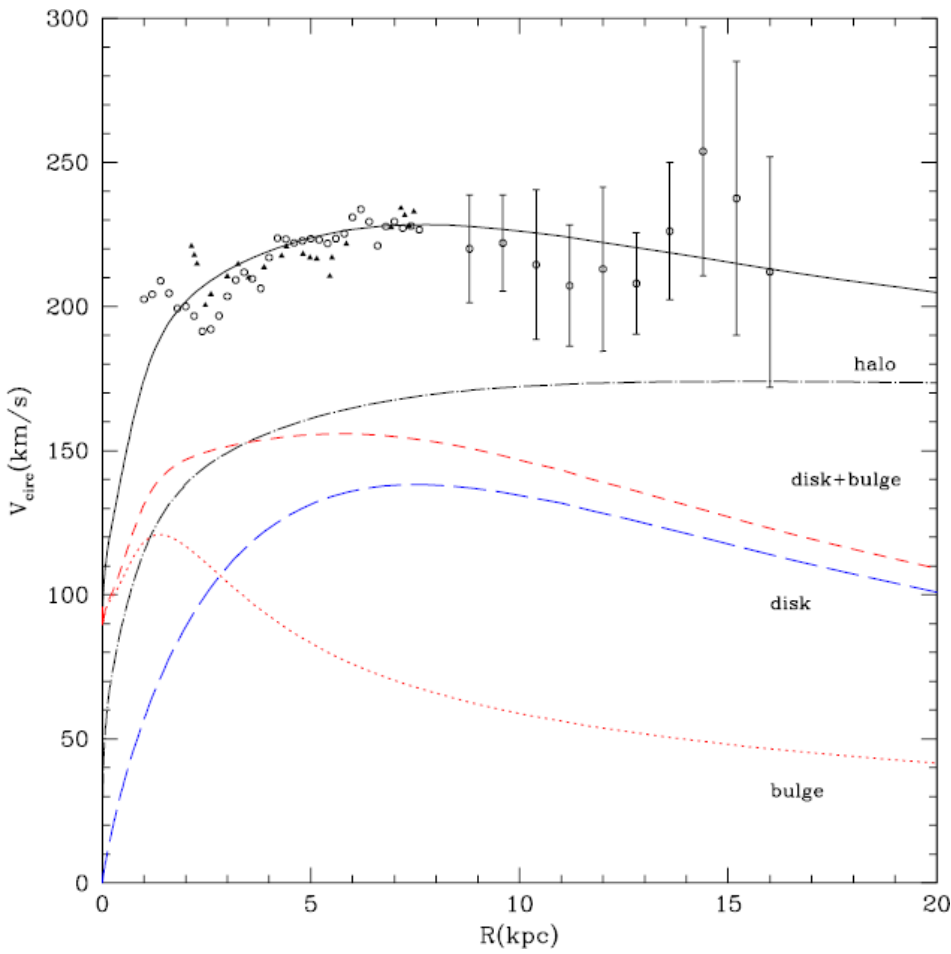
Gas height

UGC7321	$3 \times 10^9 M_{\odot}$	300 pc	580 pc
IC2233	$10^{10} M_{\odot}$	330 pc	800 pc
M33	$5 \times 10^{10} M_{\odot}$	250 pc	120 pc
Milky Way	$10^{12} M_{\odot}$	300 pc	150 pc



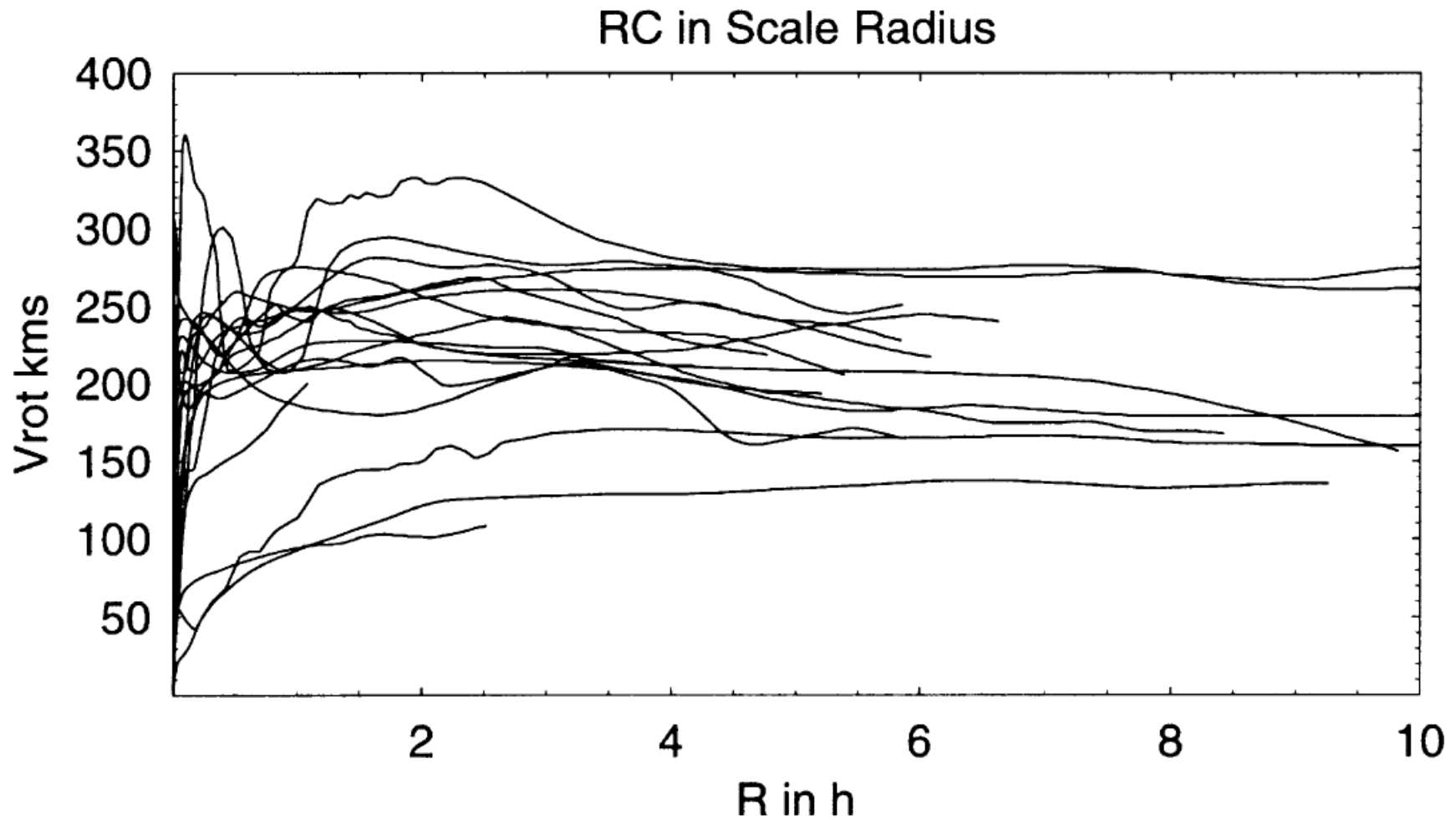
Disk of the Milky Way

- Milky Way has a “flat” rotation curve, just like many (but not all) spiral galaxies.



Galactic Rotation Curves

- Rotation curves are like people, they are all different.



Disk Dynamics



Disks are complex!

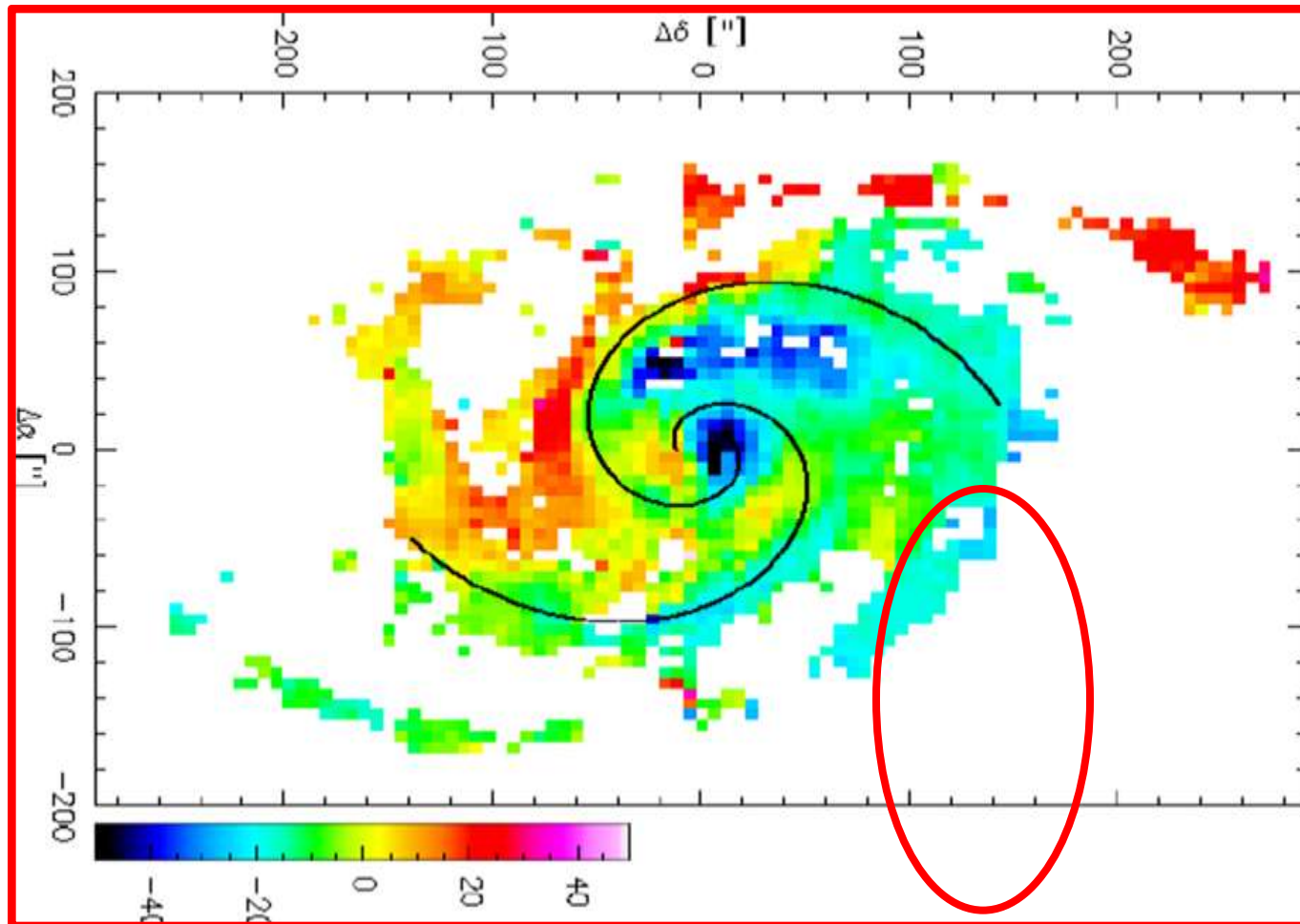
Important Lesson

Rotation velocity \neq Circular velocity

- Spiral waves are shocks, in them gas velocity changes abruptly – hence, gas does not move on circular orbits in spiral arms.
- Spirals arms are not the only waves in the disks – there exist other waves (bending modes, bars, warps, etc).
- Some of famous “controversies” about spiral galaxies (cores vs cusps, a 4-letter word) may be simply due to that crucial fact.

Important Lesson

- Non-circular motions typically reach 10-20%.



Painting by Stars



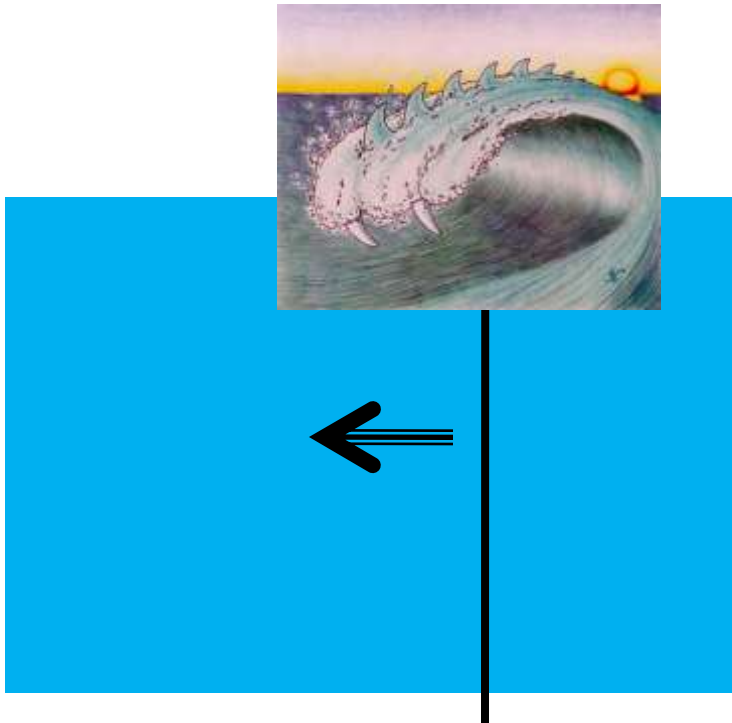
What do you see?

- Spiral arms.
- Cold dust is located along the inner edge.
- Heated dust is just outside it.
- Young (=blue) stars are outside hot dust.
- Diffuse gas is even further.



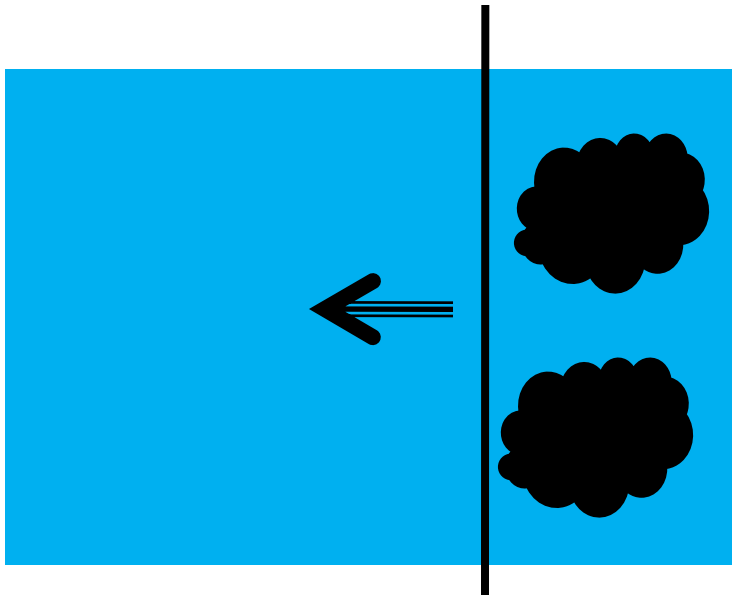
Spiral Density Waves

- Spiral arms are ***density waves***: they are not static objects, gas flows through them in a cycle of galactic ecology:
 - A. *Diffuse gas*** gets hit by a wave...



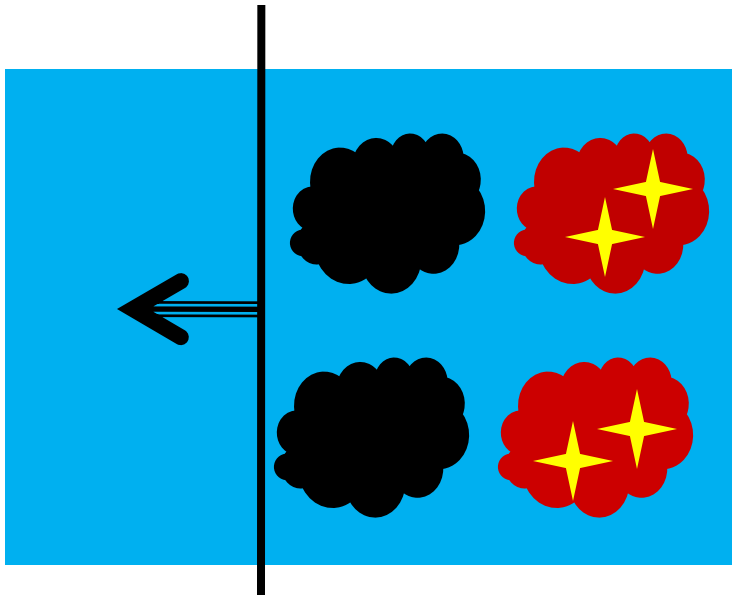
Spiral Density Waves

- Spiral arms are ***density waves***: they are not static objects, gas flows through them in a cycle of galactic ecology:
 - B.*** ...compresses, cools down, and forms cold ***molecular clouds***;



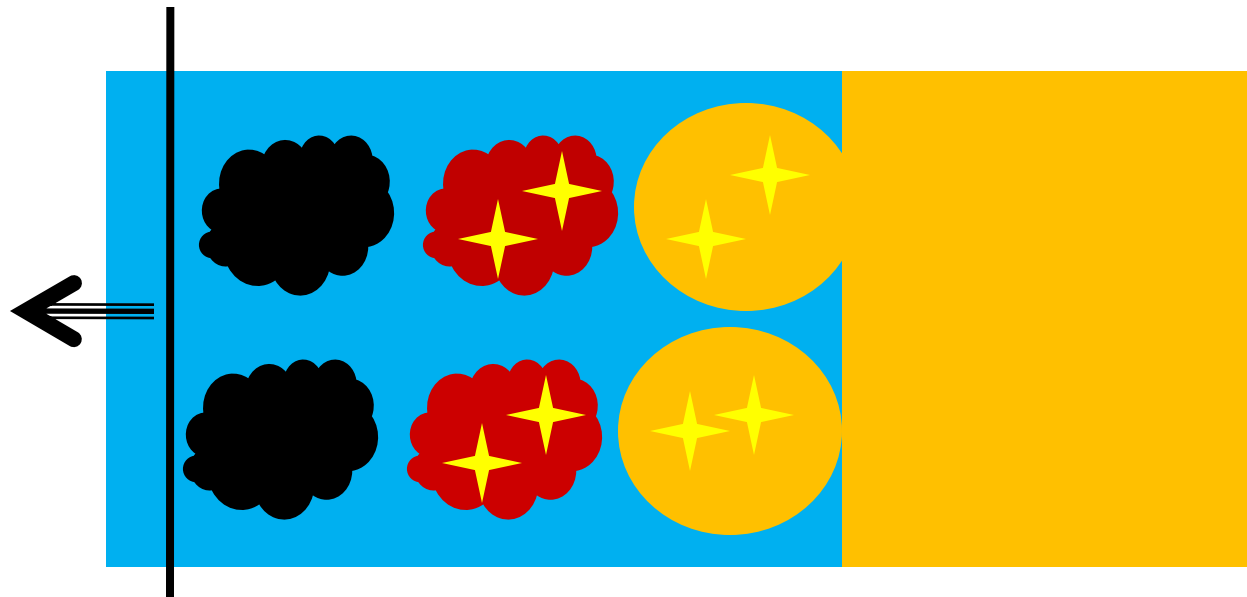
Spiral Density Waves

- Spiral arms are ***density waves***: they are not static objects, gas flows through them in a cycle of galactic ecology:
 - C. Stars** begin to form in molecular clouds, heating the gas and dust (but the wave goes on and on...)



Spiral Density Waves

- Spiral arms are ***density waves***: they are not static objects, gas flows through them in a cycle of galactic ecology:
 - D.*** Eventually, molecular gas gets heated by UV radiation and supernova explosions, turning into ***coronal gas***.



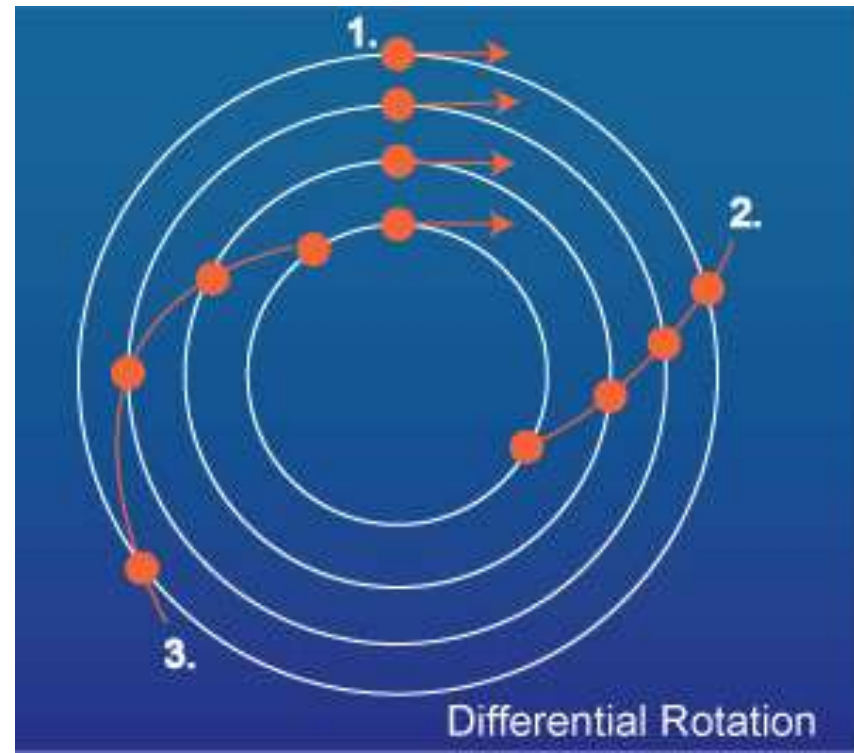
Spiral Density Waves

- Spiral arms are ***density waves***: they are not static objects, gas flows through them in a cycle of galactic ecology:
 - E.*** After the wave passed, coronal gas gradually cools into ***diffuse gas***, until the next spiral wave comes...

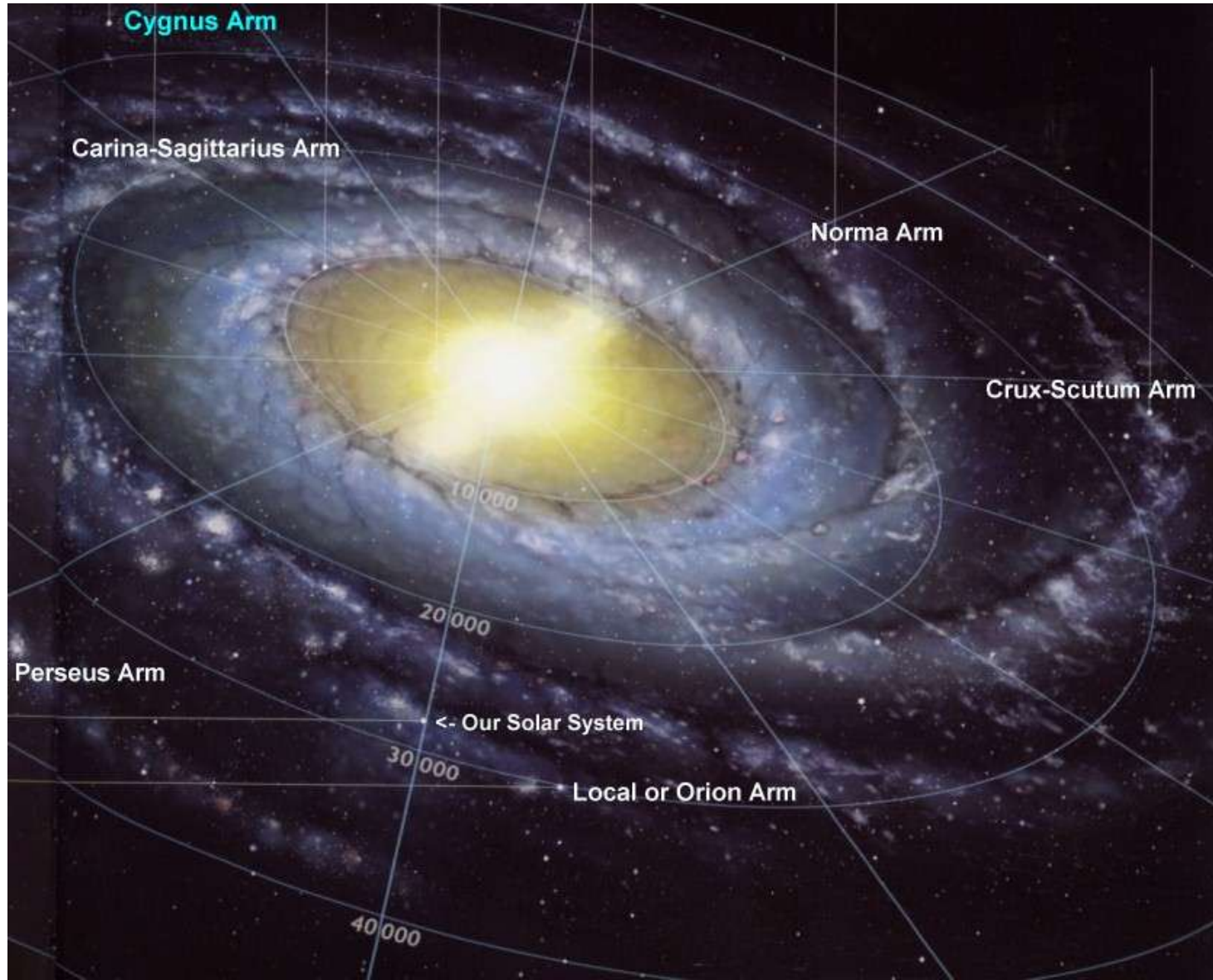


Why A Spiral?

- **Differential rotation** tends to stretch any pattern into a spiral.
- Rotation curve is flat, so stars closer to the center take less time to go around a smaller circle.
- A density wave gets ahead in the central region of a galaxy and falls behind on the outside.



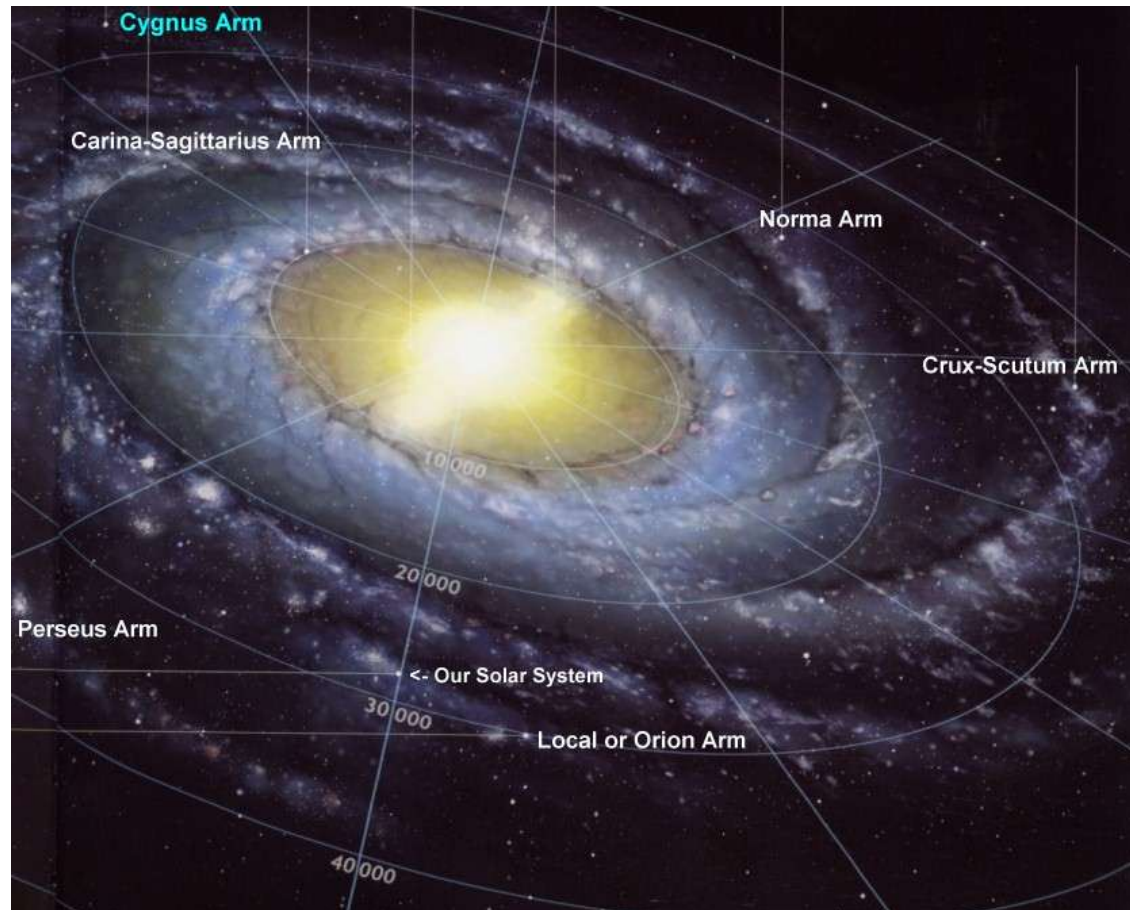
Our Spiral Arms



Quiz:

Which spiral arm did the Sun formed in?

- **A** Orion
- **B** Perseus
- **C** Normal
- **D** Carina-Sagittarius
- **E** Crux-Scutum
- **F** Cygnus



The Grandest Idea in Astronomy

- The crests of ocean waves are covered by foam.
- The crests of galactic waves are covered by new stars!



3. Disk Stability

- Studying the linear stability of gaseous disks is much easier than of stellar disks.

$$\Sigma(t, R) = \bar{\Sigma}(R) + \Delta\Sigma(t, R)$$

$$\Delta\Sigma \propto \exp(-i\omega t + i \int^R k(R) dR)$$

- After some algebra (and a bit of calculus), we get a dispersion relation for *radial perturbations*:

$$\omega^2 = \kappa^2 - 2\pi G \bar{\Sigma} |k| + c_S^2 k^2$$

- $\kappa^2 \equiv R(d\Omega^2/dR) + 4\Omega^2$ is the *epicycle frequency*.

Toomre Criterion

- Disk is stable if $\omega^2 > 0$ for any k :

$$(\pi G \bar{\Sigma})^2 < \kappa^2 c_S^2$$

- or, alternatively,

$$Q \equiv \frac{\kappa c_S}{\pi G \bar{\Sigma}} > 1 \equiv Q_{\text{crit}}$$

- This is called *Toomre's stability criterion* (after Alan Toomre), and Q is often called *Toomre Q (parameter)*.
- For a stellar disk the criterion is similar:

$$Q \equiv \frac{\kappa \sigma_R}{3.36 G \bar{\Sigma}} > 1$$

Toomre Criterion

- For an unstable ($Q < 1$) disk the range of unstable wavenumbers is

$$k_{\text{crit}} = \frac{\kappa}{Qc_S} \left(1 \pm \sqrt{1 - Q^2} \right)$$

$$k_{\text{fast}} = \frac{\kappa}{Qc_S}$$

- Hence, on very large ($k \rightarrow 0$) and very small ($k \rightarrow \infty$) scales the disk is stable.

Beyond Toomre

- A case of arbitrary, not only radial (i.e. axially-symmetric) perturbations was considered by Polyachenko & Polyachenko (1997JETP...85..417P)

$$Q_{\text{crit}}^2 = \frac{3\alpha^2 - 3}{2\alpha^2 - 3} > 1$$

$$\alpha^2 = \frac{2\Omega}{R|d\Omega/dR|}$$

- For a flat rotation curve $\alpha^2 = 2$ and

$$Q_{\text{crit}} = \sqrt{3}$$

Beyond Toomre

- A disk with finite thickness was considered by Begelman & Shlosman (2009ApJ...702L...5B):

$$\omega^2 = \kappa^2 - 2\pi G \frac{\bar{\Sigma}|k|}{1 + |k|h} + c_S^2 k^2$$

- For small scales ($kh \gg 1$) and $\bar{\Sigma} = 2\bar{\rho}h$, this becomes

$$\omega^2 \approx c_S^2 k^2 - 4\pi G \bar{\rho}$$

which should be familiar to everyone...

Dangers Of Modeling Disks

- How one would go about simulating a self-gravitating gaseous disk (a gas-dominated galaxy or a circumnuclear disk)?
- Let's set up a axially-symmetric disk with a given $\Sigma(R)$, put it into a full hydrodynamic code (with cooling, star formation, feedback, etc).
- Ready, set, go! What do you get as the result?



Dangers Of Modeling Disks

- Cooling times are often short. A homogeneous disk can rapidly cool to the state with $Q \ll 1$ and fragment into clumps with sizes

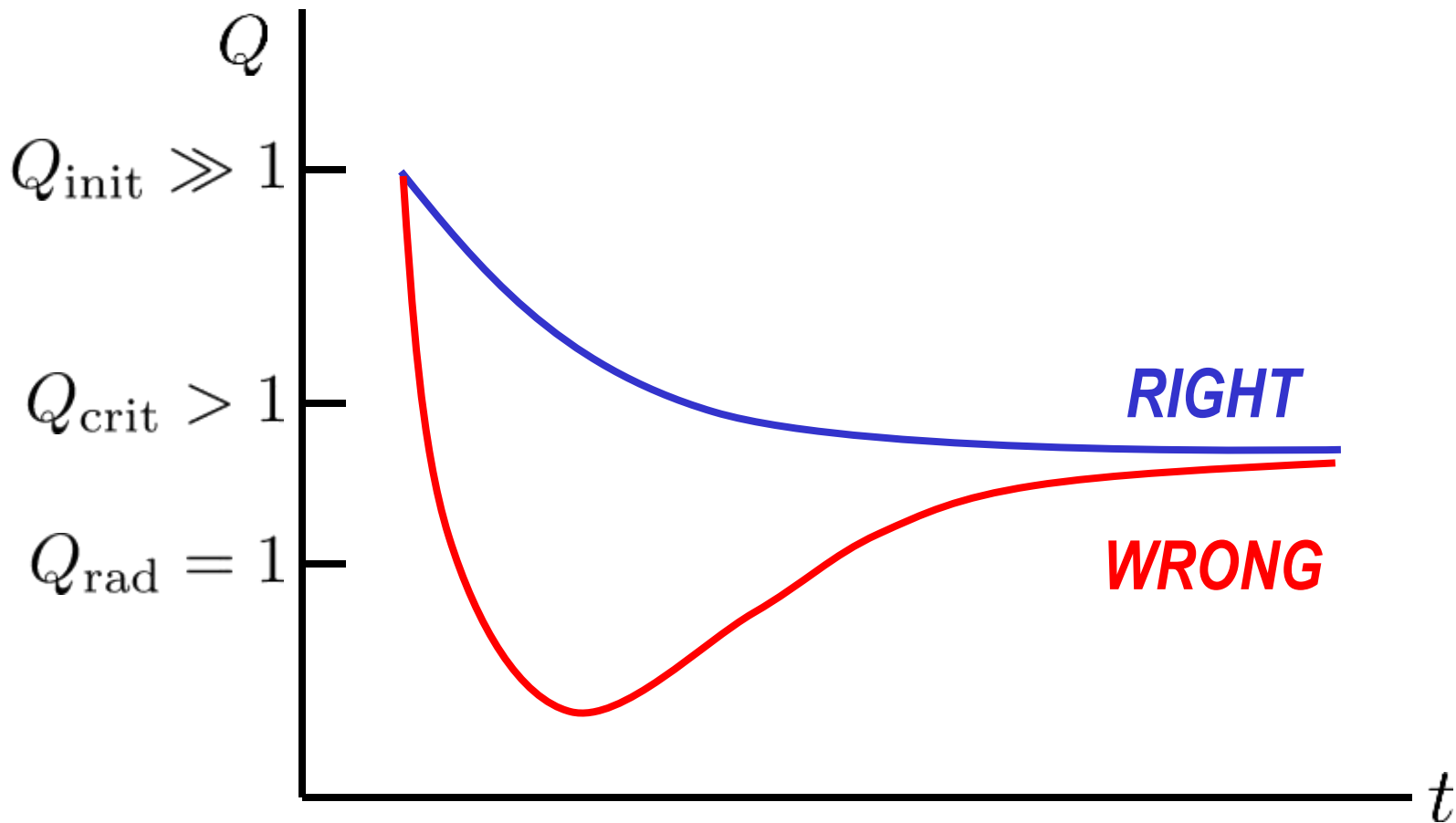
$$R \approx \lambda_{\text{fast}} = 2\pi Q \frac{c_S}{\kappa}$$

- However, a cold (i.e. violently unstable) homogenous disk is ***unphysical*** – there is no physical process that can create such a system.
- Let's start with an initially stable disk ($Q \gg 1$)...

Dangers Of Modeling Disks

- Disk becomes unstable gradually (say, by accreting mass or by gradually losing turbulent support).
- At some moment Q reaches $Q_{\text{crit}} > 1$ (which will depend on the density profile of the disk).
- At that moment some non-radial perturbations become unstable and grow to become non-linear waves, then shocks. Shocks in a differentially rotating disk become oblique and generate turbulence or turbulence-like cascade.
- Turbulence will provide extra support to the disk and limit fragmentation to $R \sim 2\pi\sigma_t/\kappa$

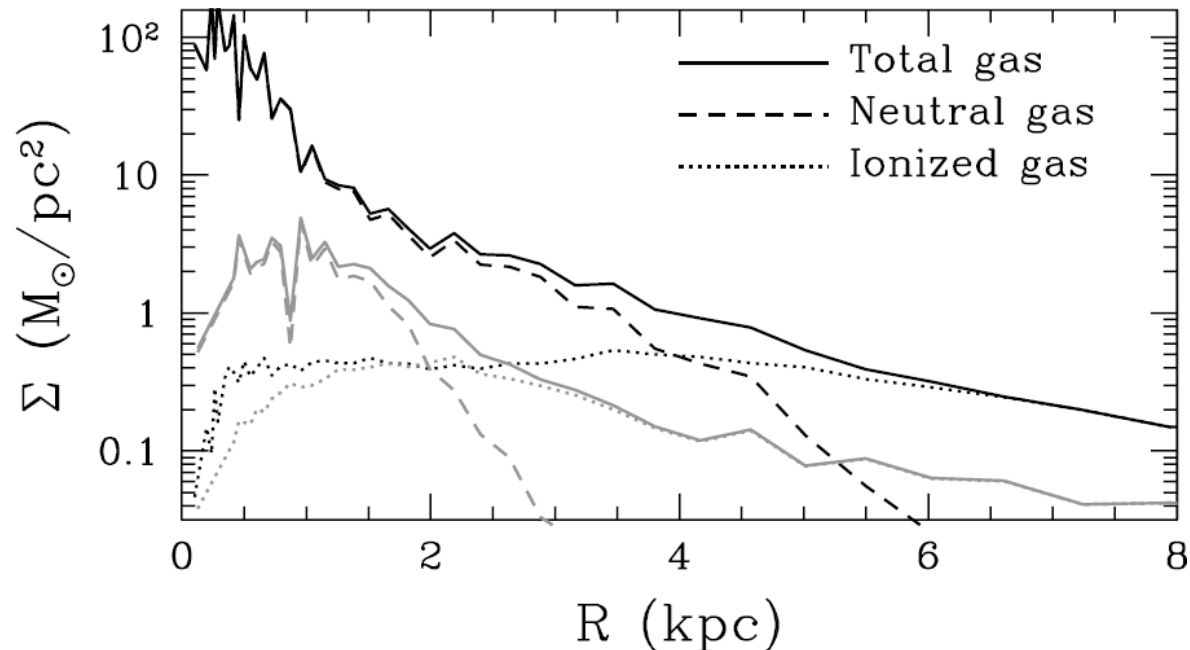
Dangers Of Modeling Disks



If in your simulations you ever get $Q \ll 1$, you are probably doing something wrong...

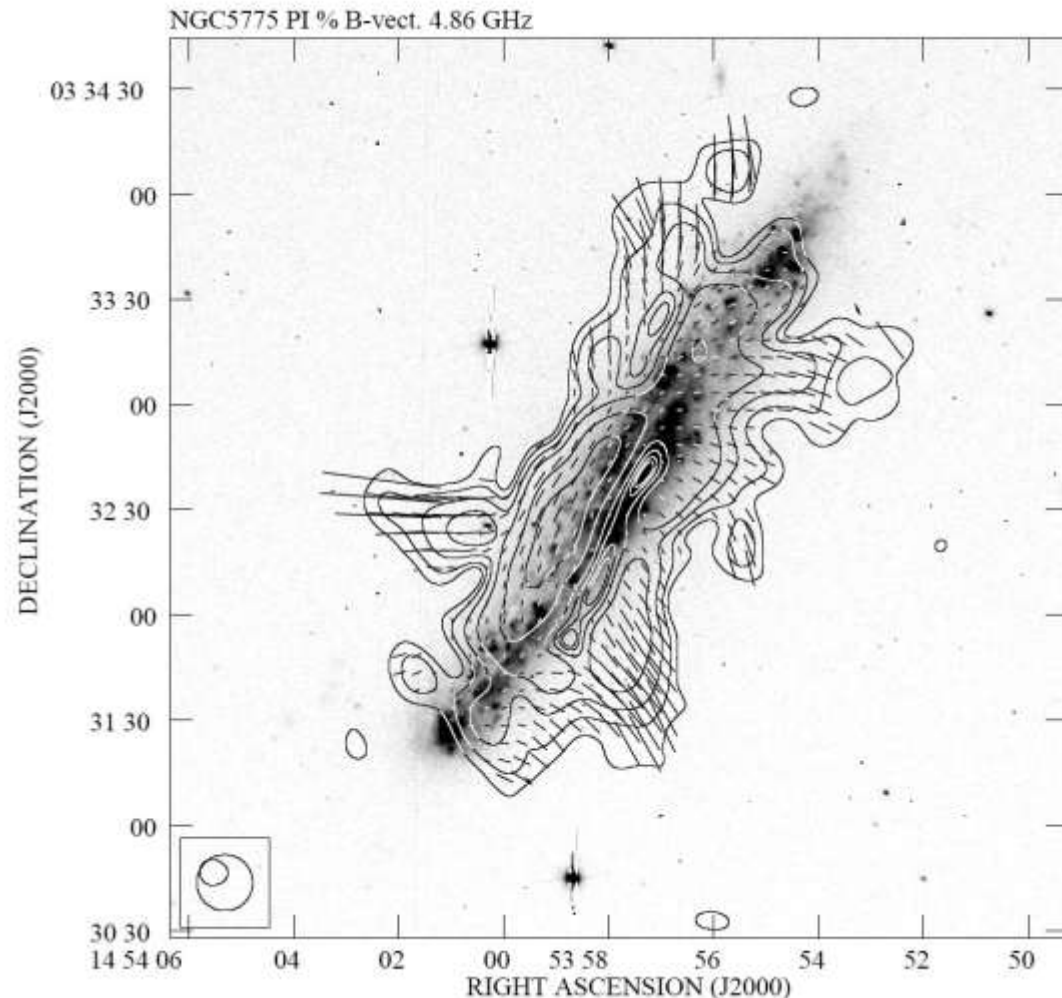
4. Reynolds Layer

- Recall, no one switched the Cosmic Ionizing Background off.
- Hence, one should expect the gaseous disks to be ionized by CIB down to $N_H \sim 3 \times 10^{19} \text{cm}^{-2}$.
- Photo-ionized gas in the ISM has many names:
WIM, DIG, Reynolds layer



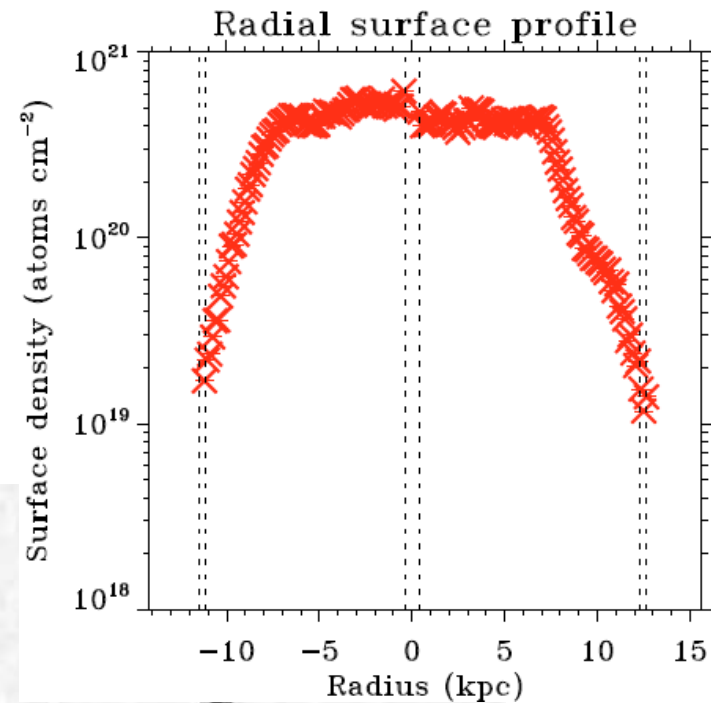
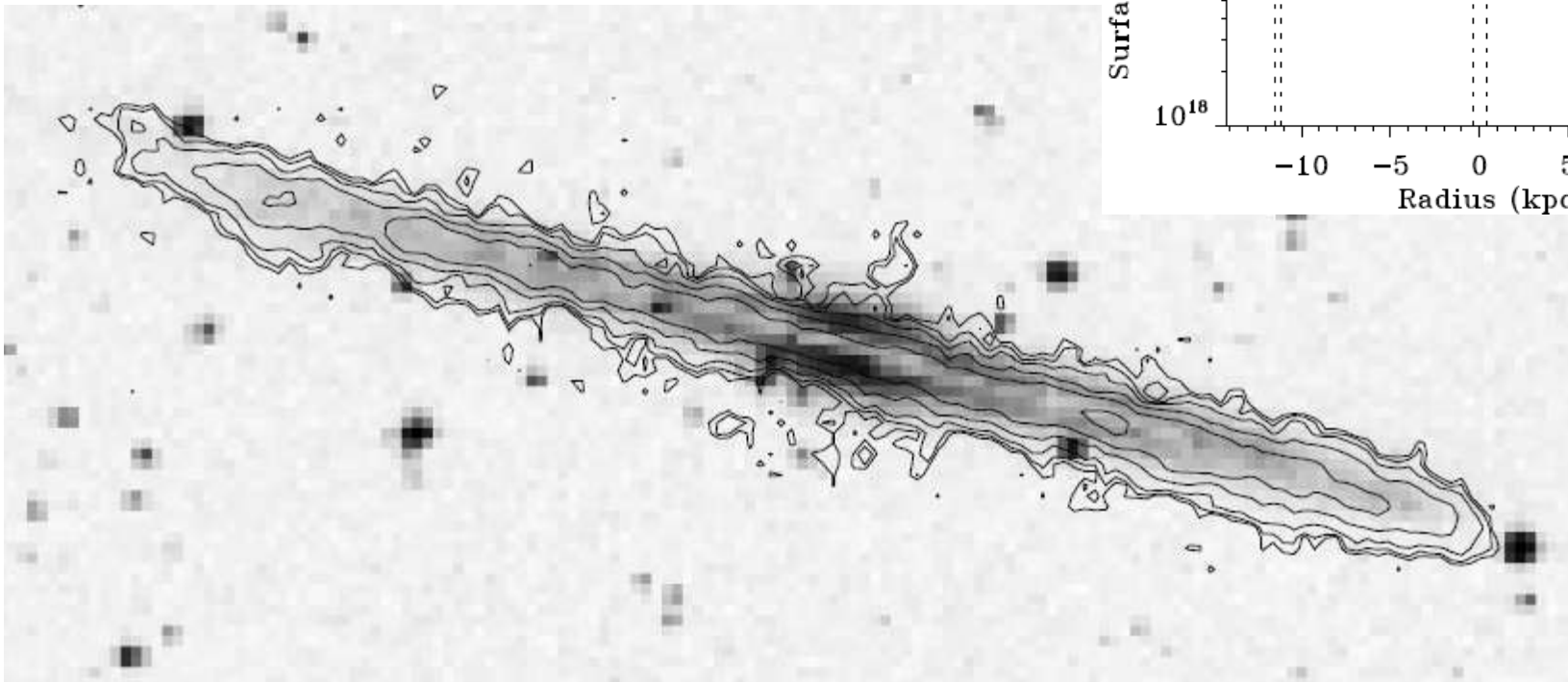
WIM In Other Galaxies

- In the Milky Way WIM has $\Sigma \sim 1 M_{\odot}/\text{pc}^2$.
- WIM/DIG/RL is also observed in external galaxies.
- Details of the main ionization source (CIB, stars, CR) are still unknown.



Disk Edges

- HI disks are often observed to have rather sharp outer edges.
- What could cause them?



5. From Atomic To Molecular Gas

- Stars (at least most of them) form from molecular gas.
- Hence, the transition from atomic to molecular gas is a necessary condition for (the bulk of) star formation.

H₂ Chemistry 101

Production

- Molecular hydrogen is produced in two separate channels:
 - Numerous reactions in the gaseous phase, through rare ions H⁻ and H₂⁺.
 - Using cosmic dust as a catalyst.

H₂ Chemistry 101

Production

$$\dot{\mathcal{M}}_{\text{H}_2} = -\Gamma_D n_{\text{H}_2} - \Gamma_E n_{\text{H}_2} - \Gamma_{LW} n_{\text{H}_2} - k_7 n_{\text{H}_2} n_{\text{HII}} - k_8 n_e n_{\text{H}_2} - k_9 n_{\text{HI}} n_{\text{H}_2} - k_{10} n_{\text{H}_2} n_{\text{H}_2} - k_{11} n_{\text{HeI}} n_{\text{H}_2} - k_{23} n_e n_{\text{H}_2} - k_{24} n_{\text{HeII}} n_{\text{H}_2} - k_{25} n_{\text{HeII}} n_{\text{H}_2} + k_2 n_{\text{H}^-} n_{\text{HI}} + k_4 n_{\text{H}_2^+} n_{\text{HI}} + k_{21} n_{\text{H}_2^+} n_{\text{H}^-} + k_{30} n_{\text{HI}}^3 + k_{31} n_{\text{HI}}^2 n_{\text{H}_2} + k_{32} n_{\text{HI}}^2 n_{\text{HeI}},$$

$$\dot{\mathcal{M}}_{\text{H}_2^+} = -\Gamma_B n_{\text{H}_2^+} - \Gamma_C n_{\text{H}_2^+} + \Gamma_D n_{\text{H}_2} - k_4 n_{\text{HI}} n_{\text{H}_2^+} - k_6 n_e n_{\text{H}_2^+} - k_{21} n_{\text{H}^-} n_{\text{H}_2^+} - k_{22} n_{\text{H}^-} n_{\text{H}_2^+} + k_3 n_{\text{HI}} n_{\text{HII}} + k_7 n_{\text{H}_2} n_{\text{HII}} + k_{16} n_{\text{HII}} n_{\text{H}^-} + k_{25} n_{\text{H}_2} n_{\text{HeII}},$$

$$\dot{\mathcal{M}}_{\text{H}^-} = -\Gamma_A n_{\text{H}^-} - k_2 n_{\text{HI}} n_{\text{H}^-} - k_5 n_{\text{HII}} n_{\text{H}^-} - k_{14} n_e n_{\text{H}^-} - k_{15} n_{\text{HI}} n_{\text{H}^-} - k_{16} n_{\text{HII}} n_{\text{H}^-} - k_{21} n_{\text{H}_2^+} n_{\text{H}^-} - k_{22} n_{\text{H}_2^+} n_{\text{H}^-} - k_{28} n_{\text{HeII}} n_{\text{H}^-} - k_{29} n_{\text{HeI}} n_{\text{H}^-} + k_1 n_e n_{\text{HI}} + k_{23} n_e n_{\text{H}_2},$$

- Gas-phase processes are slow, because H⁻ and H₂⁺ are rare. The H₂ fraction saturates at $\approx 10^{-3}$ until 3-body formation kicks in ($n \sim 10^{12} \text{cm}^{-3}$).
- H₂ formation in gas does not require any metals, and can proceed in primordial gas.

H₂ Chemistry 101

Production

$$\dot{D}_{\text{H}_2} = R_D D_{\text{MW}} (n_{\text{HI}} + n_{\text{H}_2}) n_{\text{HI}}$$

- Formation of H₂ on dust grains is not fully understood. It is usually assumed that atomic hydrogen accumulates on grains where two atoms can find each other much more easily (young couples tend to live in cities).
- The formation rate R_D has been modeled (somewhat inconclusively) theoretically and measured observationally by Wolfire et al. (2008)

$$R_D \approx D_{\text{MW}} \times 3.5 \times 10^{-17} \text{ cm}^2$$

H₂ Chemistry 101

Destruction

- Molecular hydrogen is destroyed by
 - Collision at $T > 5,000\text{K}$;
 - UV radiation in the Lyman-Werner band (11.3 – 13.6 eV);
 - Ionizing radiation ($> 13.6\text{ eV}$) - although this is often not important.
- Molecular clouds only exist because of shielding.



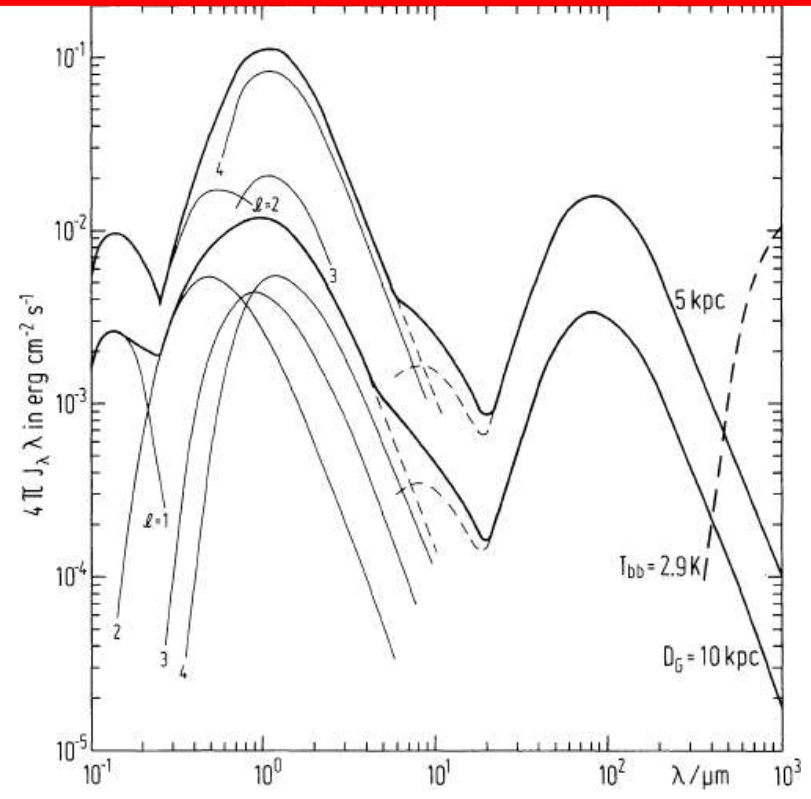
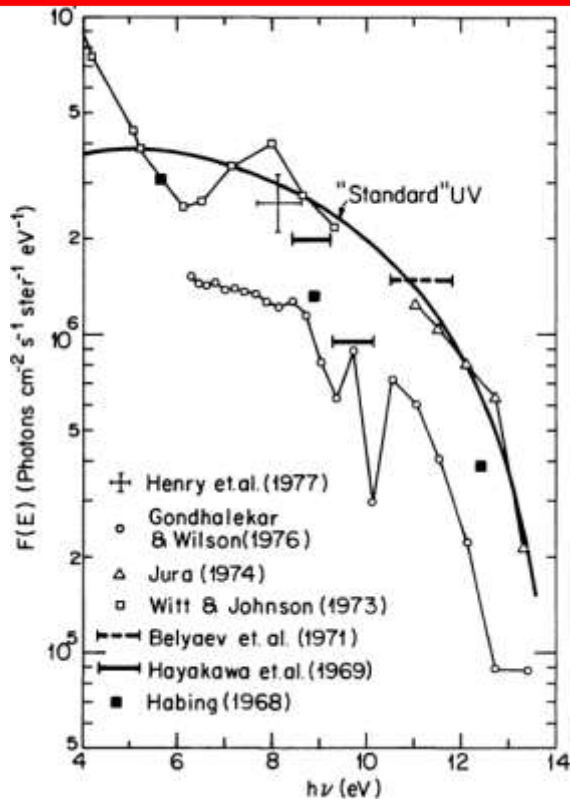
H₂ Chemistry 101

Interstellar Radiation Field

- Interstellar Radiation Field (ISRF) is not measured directly, it is *modeled*.

Draine (1978ApJS...36..595D)

Mathis et al (1983A&A...128..212M)



H₂ Chemistry 101

Interstellar Radiation Field

- In the solar neighborhood $J_0 \approx 10^6 \text{ phot/cm}^2/\text{s/eV/rad}$, but in the Galaxy the radiation field changes with the distance to the center. At the center it is up to 10 times higher than around the Sun.
- Just like masses and luminosities are convenient to measure in solar units, in galactic studies it is convenient to measure the radiation field and other quantities (like dust abundance) in the Milky Way units. Hence, hereafter we will use

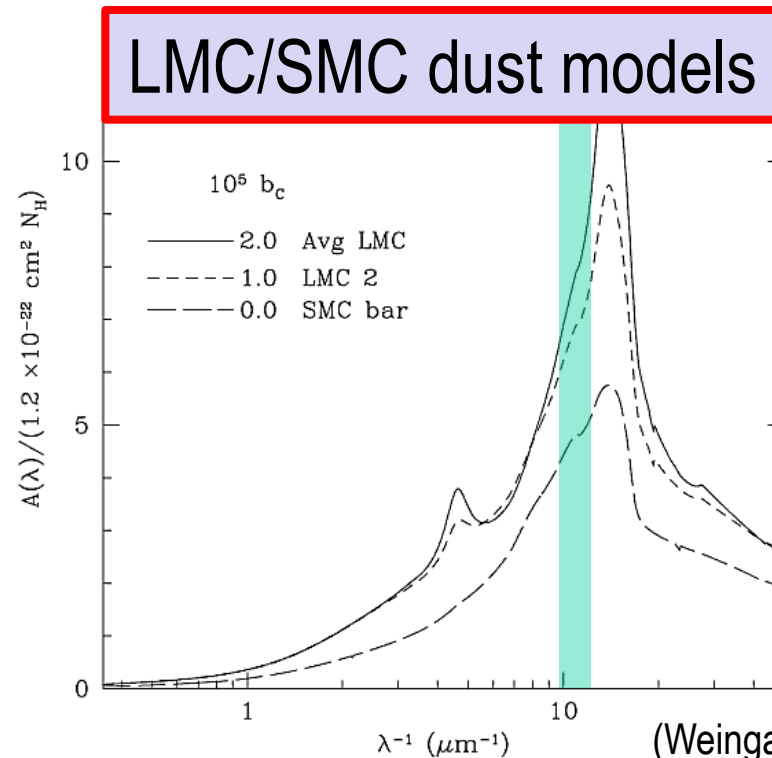
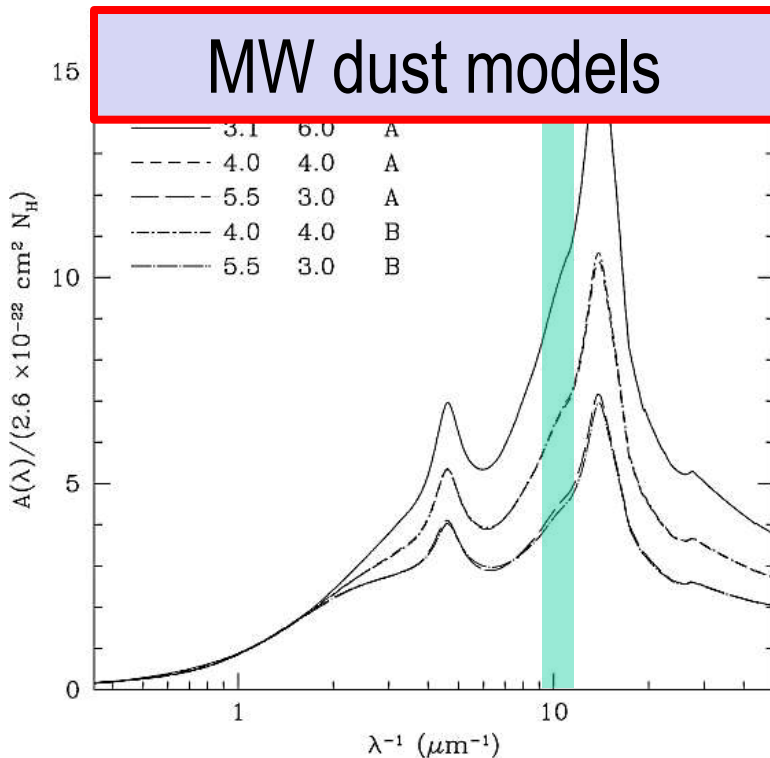
$$U_{\text{MW}} \equiv \frac{J_{\text{LW}}}{J_0}$$

- U_{MW} can be large – in $z \sim 2$ galaxies $U_{\text{MW}} = 30 - 300$.

H₂ Chemistry 101

Dust Shielding

- Dust absorbs continuum radiation over a very wide range of wavelengths, including the LW band.
- In the first approximation, the absorption in the LW band may be considered constant.



(Weingartner & Draine 2001)

H₂ Chemistry 101

Dust Shielding

- Absorption cross-section should scale with the dust abundance

$$\sigma_{\text{LW}} = D_{\text{MW}} \sigma_0$$

- and D_{MW} is the dust abundance in Milky Way units ($M_{\text{dust}}/M_{\text{H}} \approx 0.01$).

- Milky Way $D_{\text{MW}} = 1$ $\sigma_0 = 1.7 \times 10^{-21} \text{cm}^2$
- LMC $D_{\text{MW}} = 0.5$ $\sigma_0 = 1.6 \times 10^{-21} \text{cm}^2$
- SMC $D_{\text{MW}} = 0.2$ $\sigma_0 = 2.2 \times 10^{-21} \text{cm}^2$

H₂ Chemistry 101

Dust Shielding

- Continuum shielding (over a narrow band) is straightforward:

$$\Gamma = c \sum_j \int_{\nu_1}^{\nu_2} \sigma_j(\nu) \underbrace{e^{-\sigma_d(\nu) N_H} n_\nu}_{\text{radiation field}} d\nu \approx e^{-\bar{\tau}_d} \Gamma_0$$

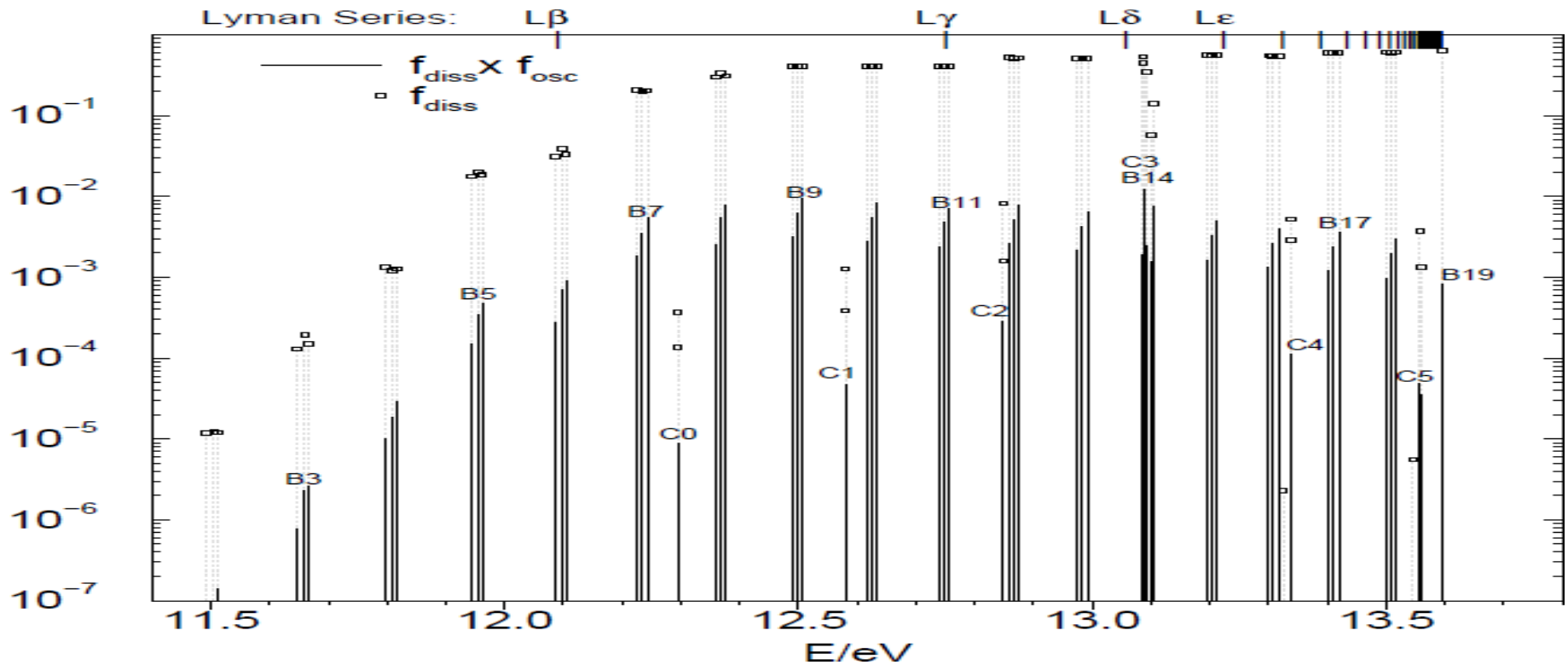
- Define a *shielding factor* S such that $\Gamma = S\Gamma_0$, hence

$$S_d(D_{\text{MW}}, N_{\text{H}}) = e^{-D_{\text{MW}} \sigma_0 N_{\text{H}}}$$

H₂ Chemistry 101

Self-shielding

- Self-shielding of H₂ is much more messy.
- LW band consists of numerous lines of various strengths. Absorbing a photon in one of those lines may or may not lead to the destruction of the H₂ molecule.



H₂ Chemistry 101

Self-shielding

- Line shielding is much more complex:

$$\Gamma = c \sum_j \int_{\nu_1}^{\nu_2} \sigma_j(\nu) \underbrace{e^{-\sigma_j(\nu) N_{\text{H}_2} n_\nu}}_{\text{radiation field}} d\nu \approx \sum_j e^{-\bar{\tau}_j} \Gamma_{0,j}$$

Some lines are shielded, some are not

- Hence $S_{\text{H}_2}(N_{\text{H}_2})$ is much harder to compute.
- $S_{\text{H}_2}(N_{\text{H}_2})$ should fall much slower than an exponential at high N_{H_2} since weakest lines will remain optically thin way after stronger lines saturate.

H₂ Chemistry 101

DB96+

- A commonly used formula for S_{H_2} is from Draine & Bertoldi (1996ApJ...468..269D):

$$S_{\text{H}_2} = \frac{0.965}{(1 + x/b_5)^\alpha} + \frac{0.035}{\sqrt{1 + x}} e^{-0.00085\sqrt{1+x}}$$

$$x = \frac{N_{\text{H}_2}}{5 \times 10^{14} \text{cm}^{-2}}$$

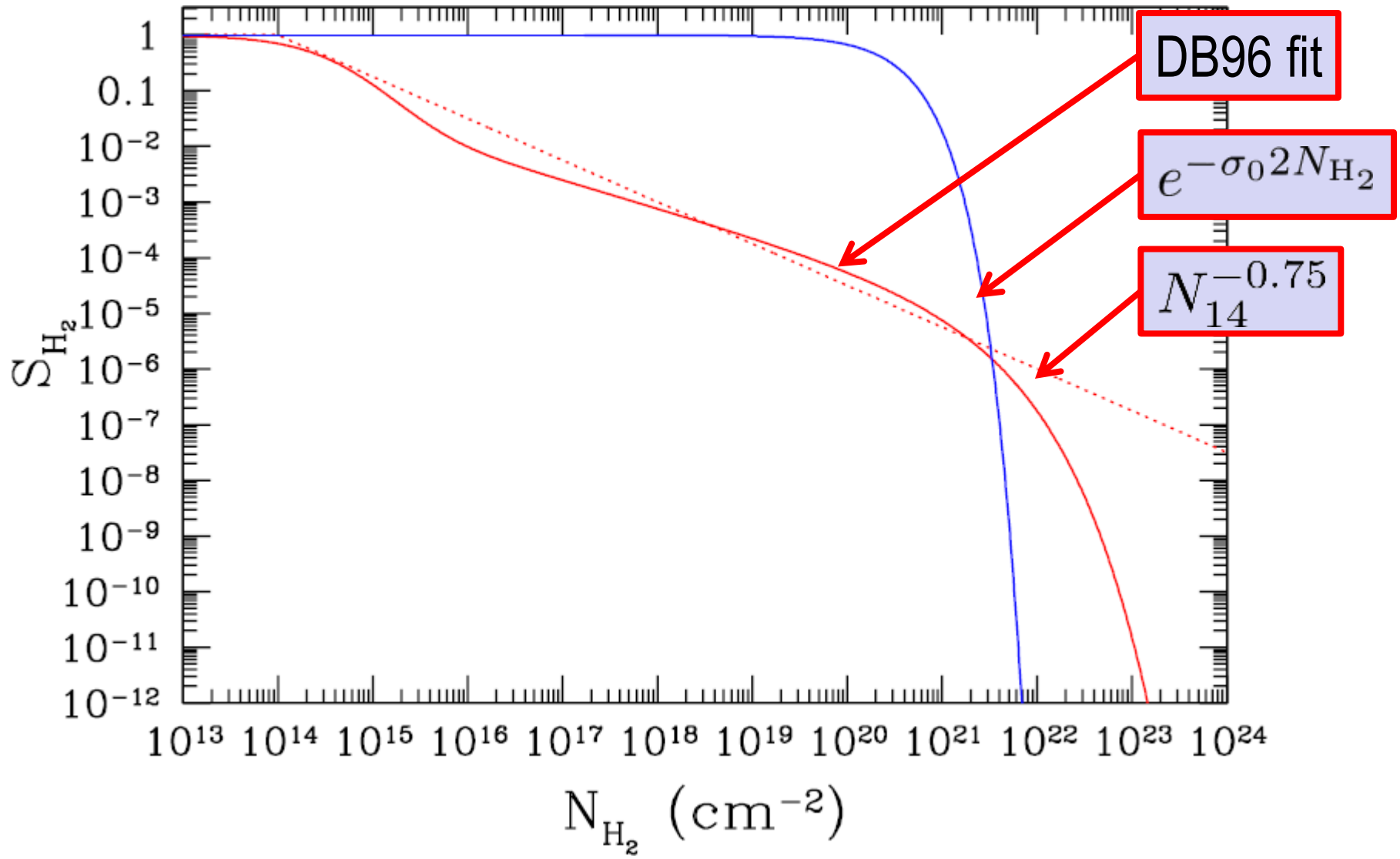
$$b_5 = \frac{b}{1 \text{ km/s}}$$

with $\alpha = 2$.

- Wolcott-Green, Haiman, & Bryan (2011MNRAS.418..838W) suggest $\alpha = 1.1$ is better at high temperatures.

H₂ Chemistry 101

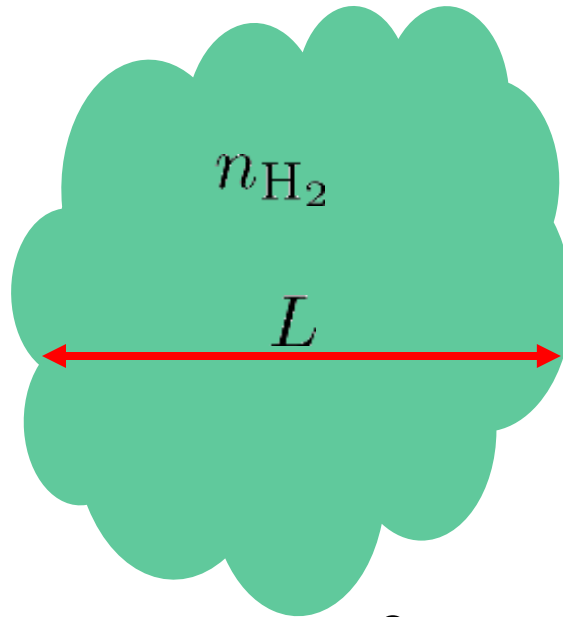
DB96+



H₂ Chemistry 101

What is N_{H_2} ?

- The last question: what is N_{H_2} in $S_{H_2}(N_{H_2})$?



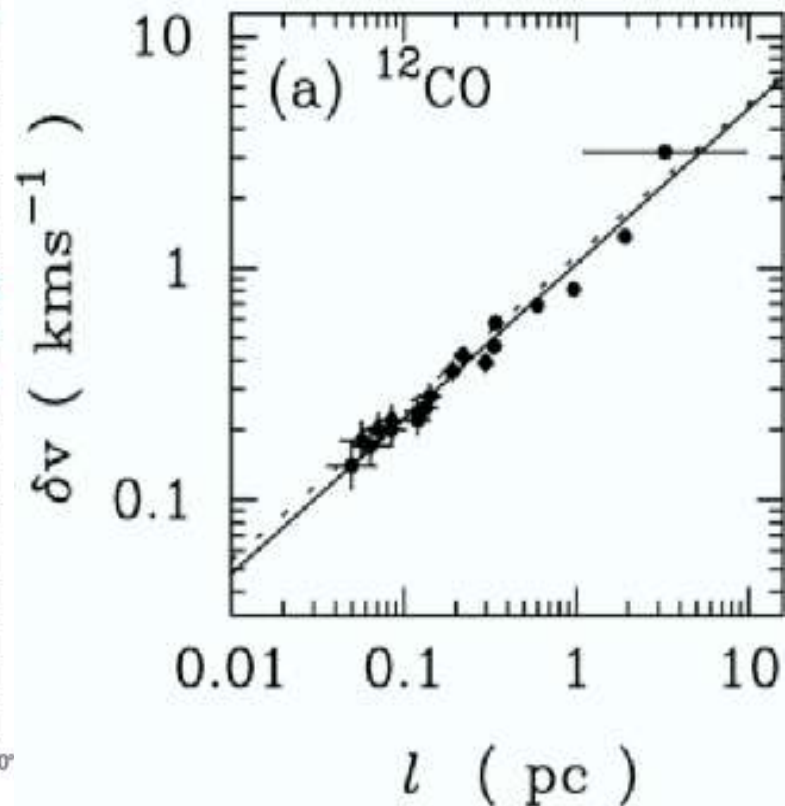
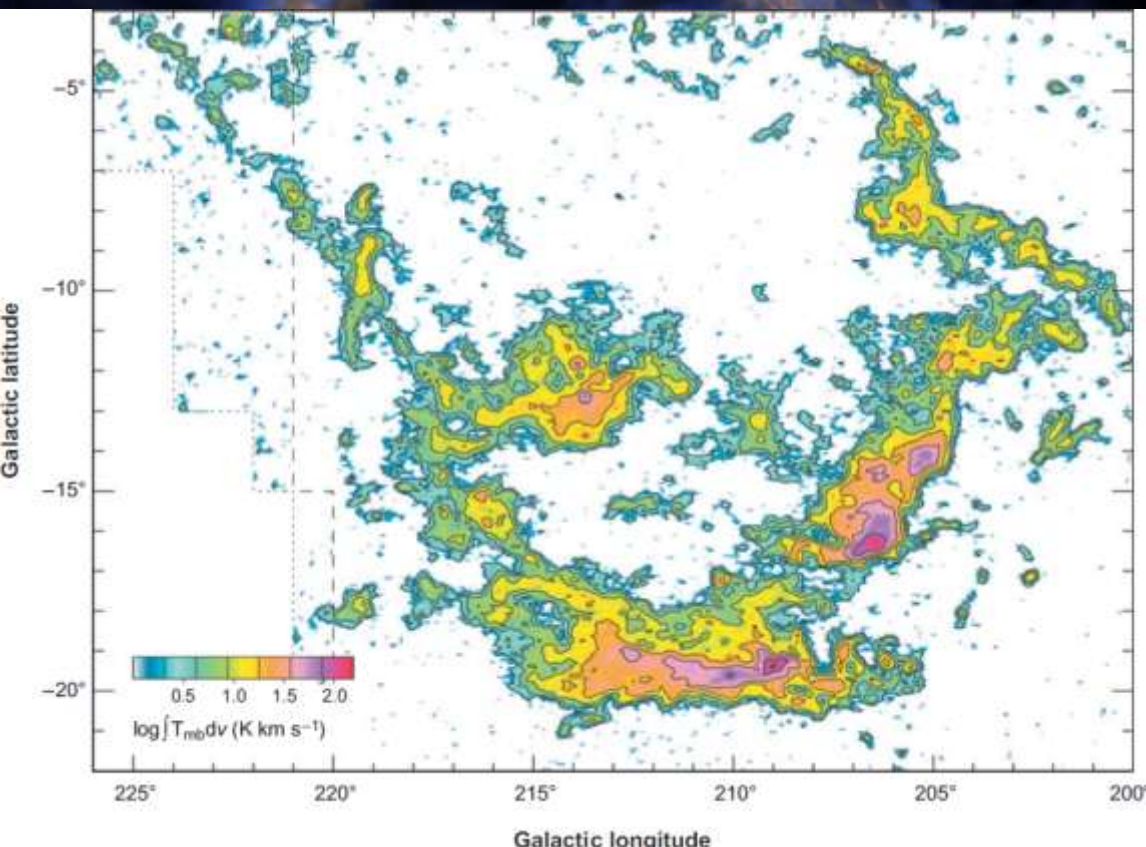
- Quiz:** is $N_{H_2} = n_{H_2} L$?
 - A. Yes
 - B. No



H₂ Chemistry 101

What is N_{H₂}?

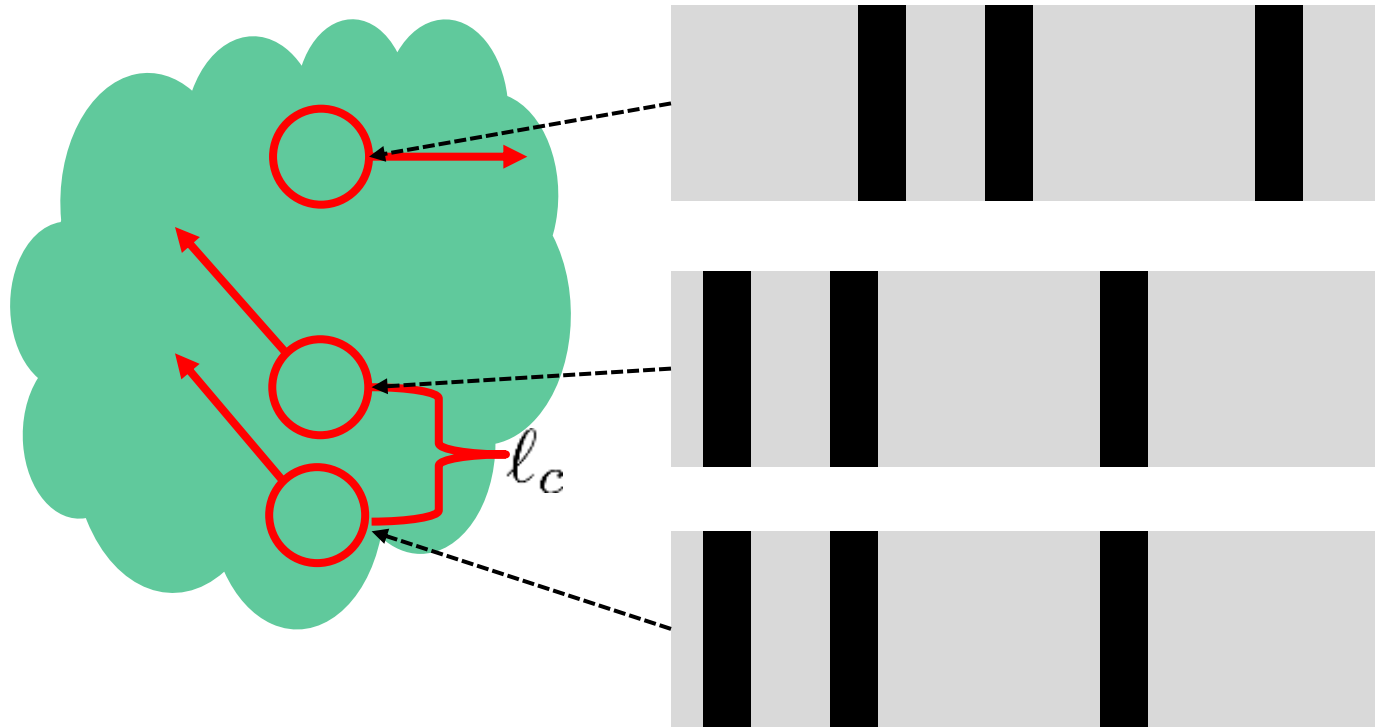
- Molecular clouds are *supersonically turbulent*. Different regions move with different velocities.



H₂ Chemistry 101

What is N_{H₂}?

- $N_{\text{H}_2} \sim n_{\text{H}_2} \ell_s$, where ℓ_s is the *sonic length* (<0.1pc).



H₂ Chemistry 101

Atomic-to-Molecular Transition

- Balancing H₂ formation and destruction rates:

$$\Gamma_{\text{LW}} S_{\text{H}_2} e^{-\sigma_{\text{LW}} N_{\text{H}}} n_{\text{H}_2} = R_{\text{D}} n_{\text{HI}} n_{\text{H}}$$

and $\Gamma_{\text{LW}} \equiv U_{\text{MW}} \Gamma_0$ is a *free-space* photo-destruction rate (i.e. a rate in the absence of any shielding).

- Hence

$$\frac{f_{\text{H}_2}}{(1 - f_{\text{H}_2})} = \frac{D_{\text{MW}}}{U_{\text{MW}}} \frac{R_0}{S_{\text{H}_2} \Gamma_0} e^{D_{\text{MW}} \sigma_0 N_{\text{H}}} n_{\text{H}}$$

- This is our master equation.

H₂ Chemistry 101

Atomic-to-Molecular Transition

Case 1: Weak radiation field

- In this case H₂ shielding dominates and dust shielding can be neglected:

$$\frac{f_{\text{H}_2}}{(1 - f_{\text{H}_2})} = \frac{D_{\text{MW}}}{U_{\text{MW}}} \frac{R_0}{S_{\text{H}_2} \Gamma_0} n_{\text{H}}$$

- With a power-law approximation to S_{H_2} :

$$\frac{f_{\text{H}_2}}{(1 - f_{\text{H}_2})} \propto \frac{D_{\text{MW}}}{U_{\text{MW}}} \frac{R_0}{\Gamma_0} (f_{\text{H}_2} n_{\text{H}} \ell_s)^{3/4} n_{\text{H}}$$

H₂ Chemistry 101

Atomic-to-Molecular Transition

- Let's say we are interested in densities at which the gas becomes 50% molecular,

$$n_{1/2} \equiv n_{\text{H}}(f_{\text{H}_2} = 1/2)$$

- In the weak field regime:

$$n_{1/2} \propto \left(\frac{U_{\text{MW}}}{D_{\text{MW}}} \right)^{4/7}$$

H₂ Chemistry 101

Atomic-to-Molecular Transition

Case 2: Strong radiation field

- In this case dust shielding dominates and self-shielding can be neglected:

$$\frac{f_{\text{H}_2}}{(1 - f_{\text{H}_2})} = \frac{D_{\text{MW}}}{U_{\text{MW}}} \frac{R_0}{\Gamma_0} e^{D_{\text{MW}} \sigma_0 N_{\text{H}} n_{\text{H}}}$$

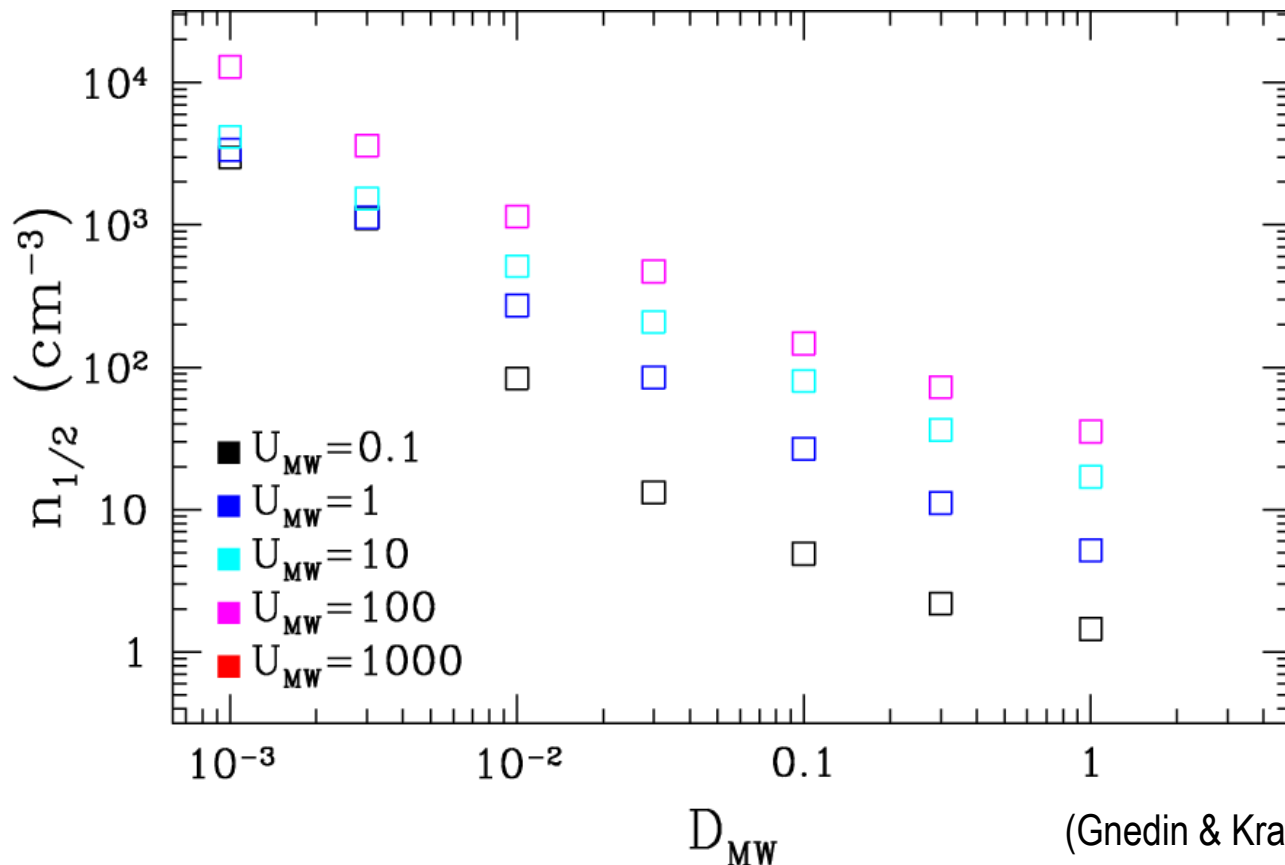
- and

$$N_{1/2} \propto \frac{1}{D_{\text{MW}}} \ln \left(\frac{U_{\text{MW}}}{D_{\text{MW}} n_{1/2}} \times \text{const} \right)$$

H₂ Chemistry 101

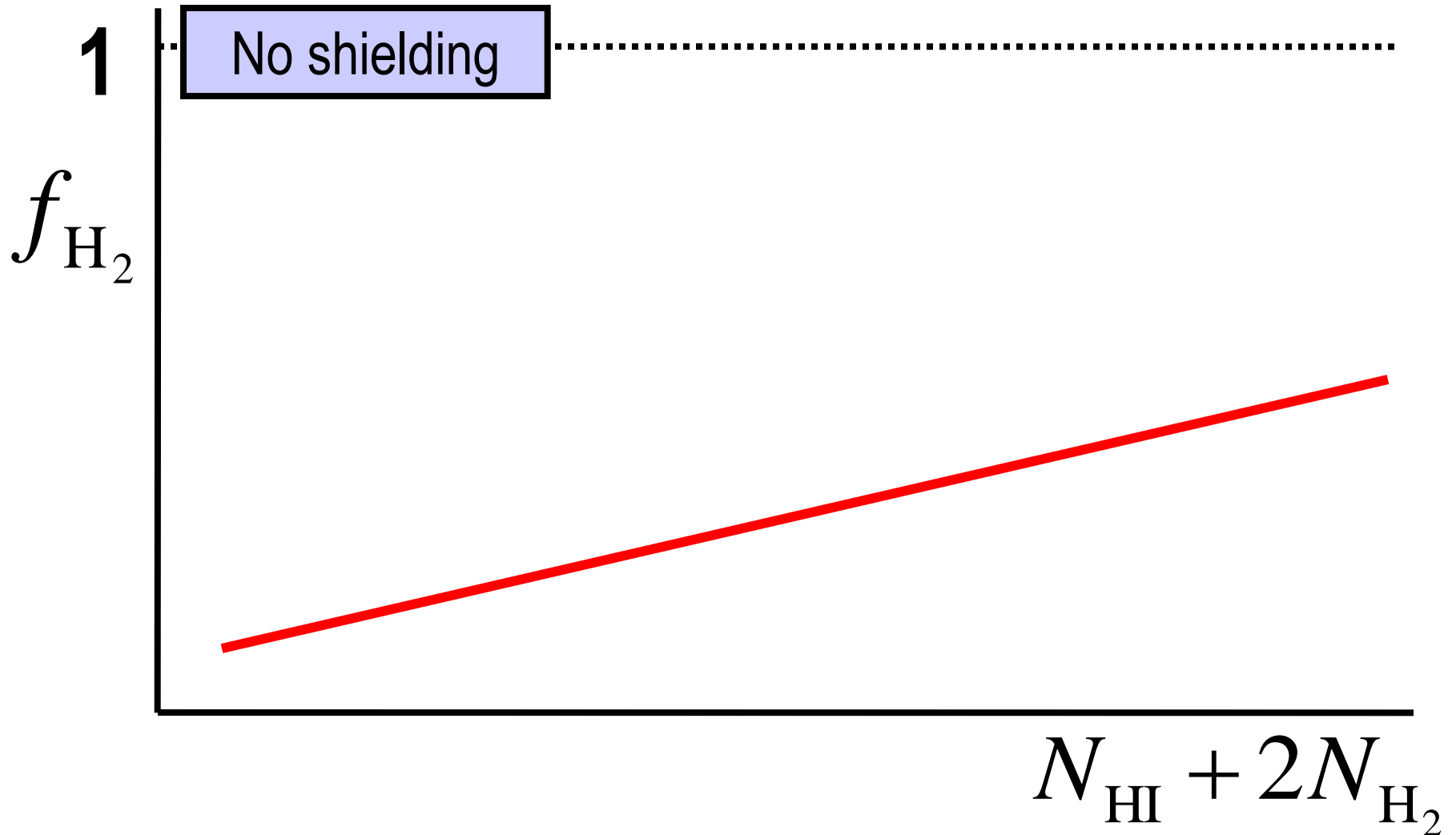
Atomic-to-Molecular Transition

- In general, there may not be a simple relation between $N_{1/2}$ and $n_{1/2}$. In galaxy formation simulations with 30-150 pc resolution such a relation exists.



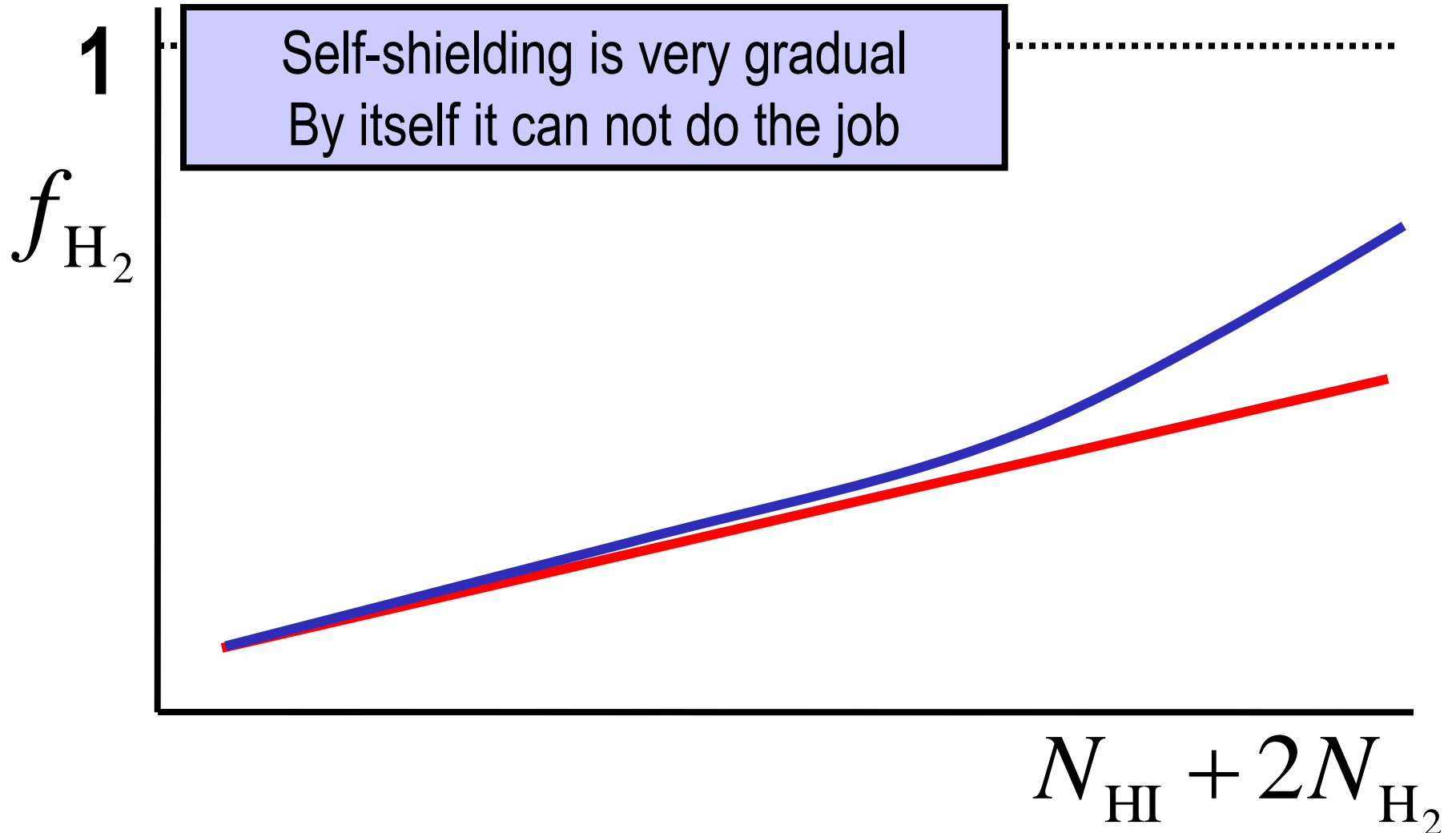
H₂ Chemistry 101

Bottom Line in Pictures



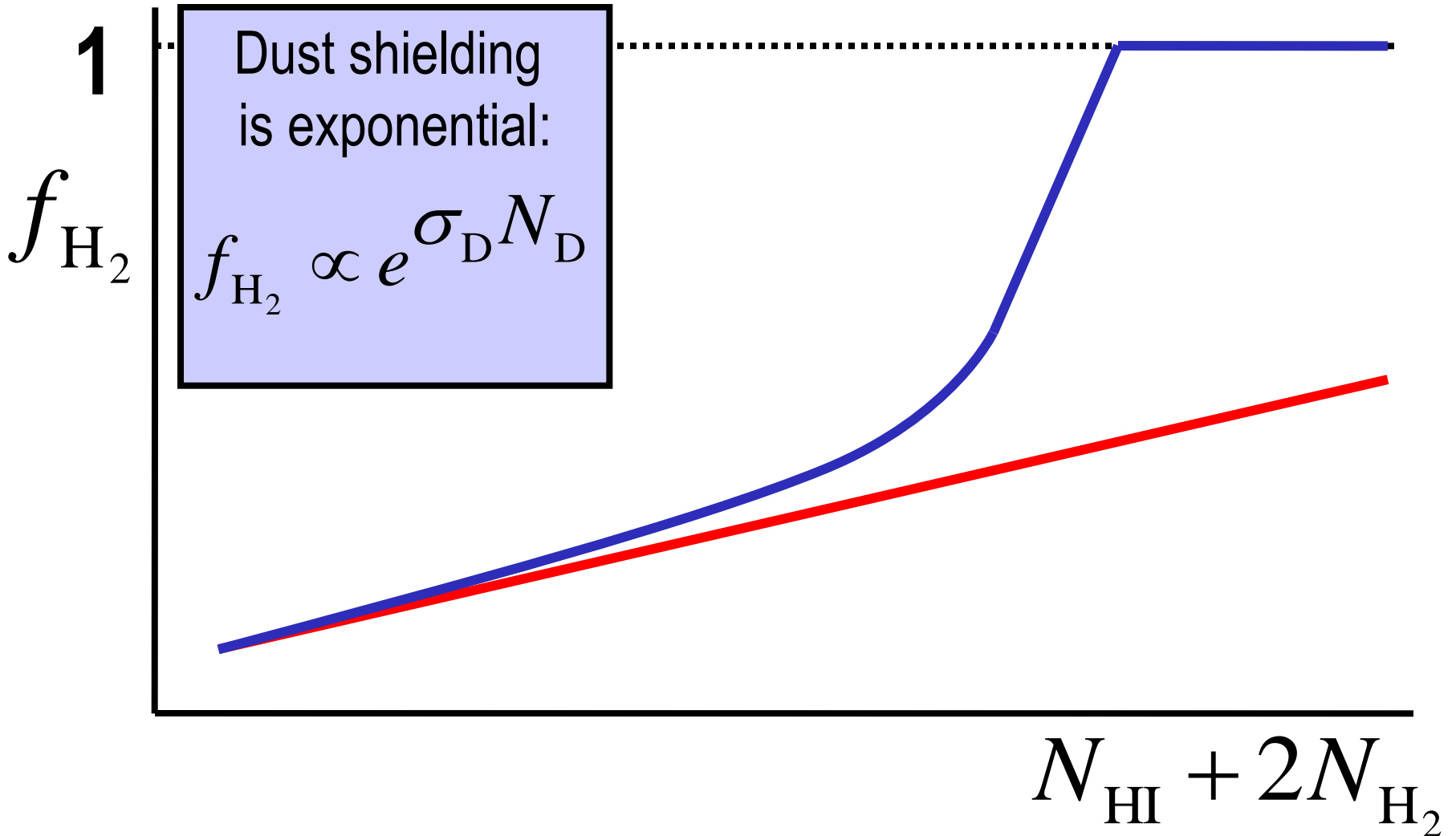
H₂ Chemistry 101

Bottom Line in Pictures



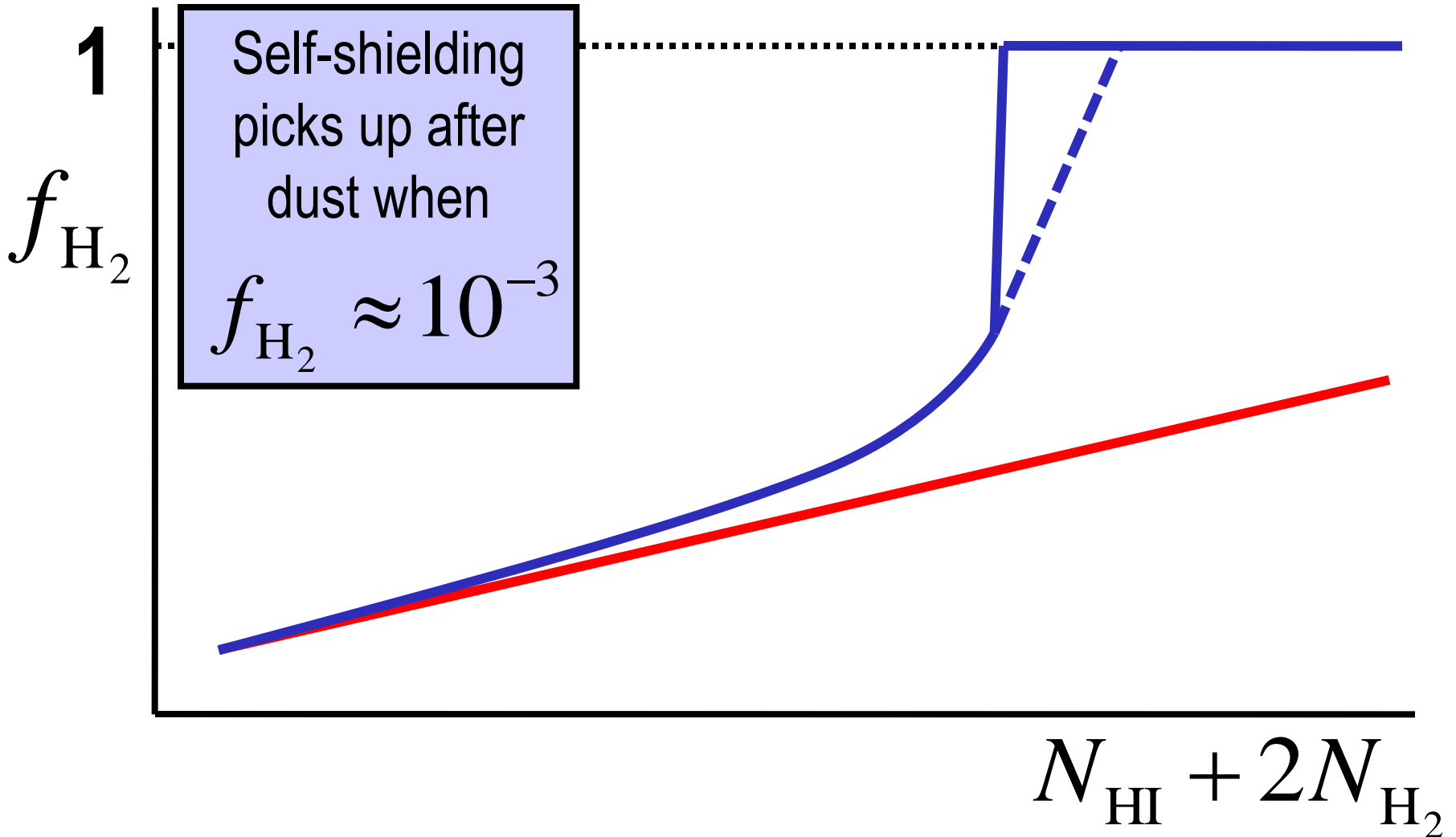
H₂ Chemistry 101

Bottom Line in Pictures



H₂ Chemistry 101

Bottom Line in Pictures

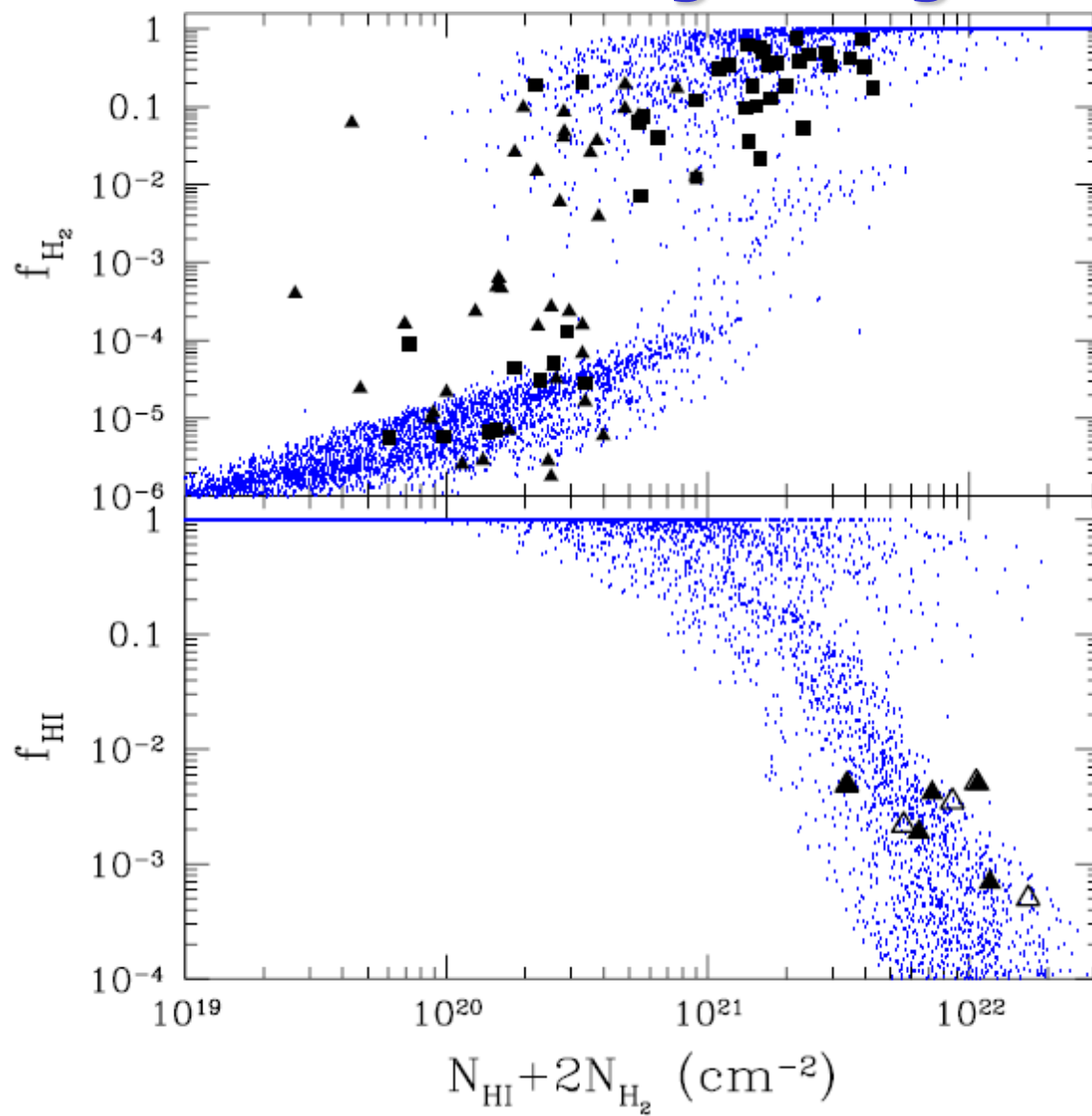


H₂ Chemistry 101 For Kids

- Dust shielding for hydrogen molecules is like a castle wall for defenders: without the wall, they are not able to withstand the assault of the UV radiation.

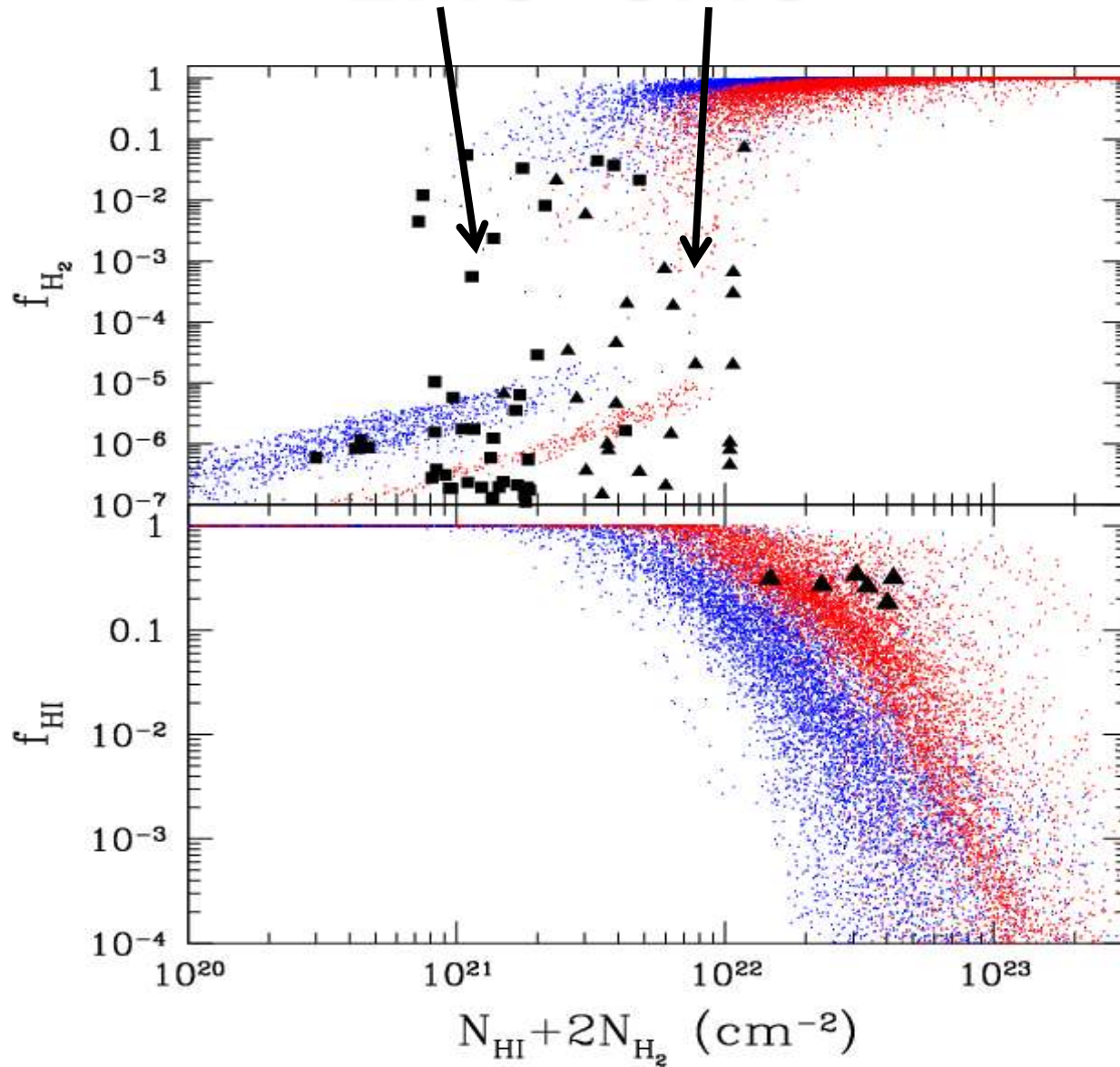


HI \rightarrow H₂ Transition: Milky Way



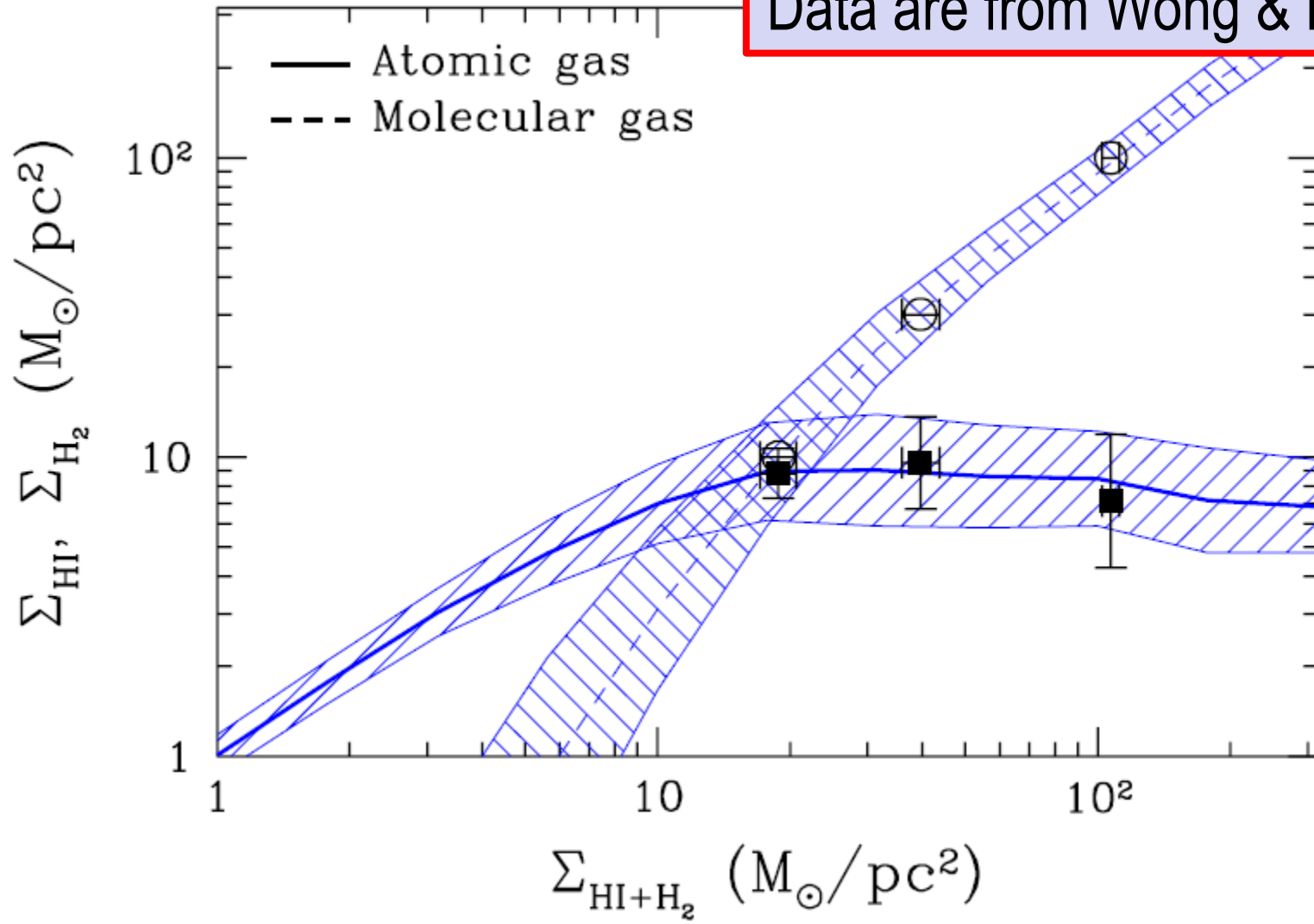


HI \rightarrow H₂ Transition: LMC+SMC



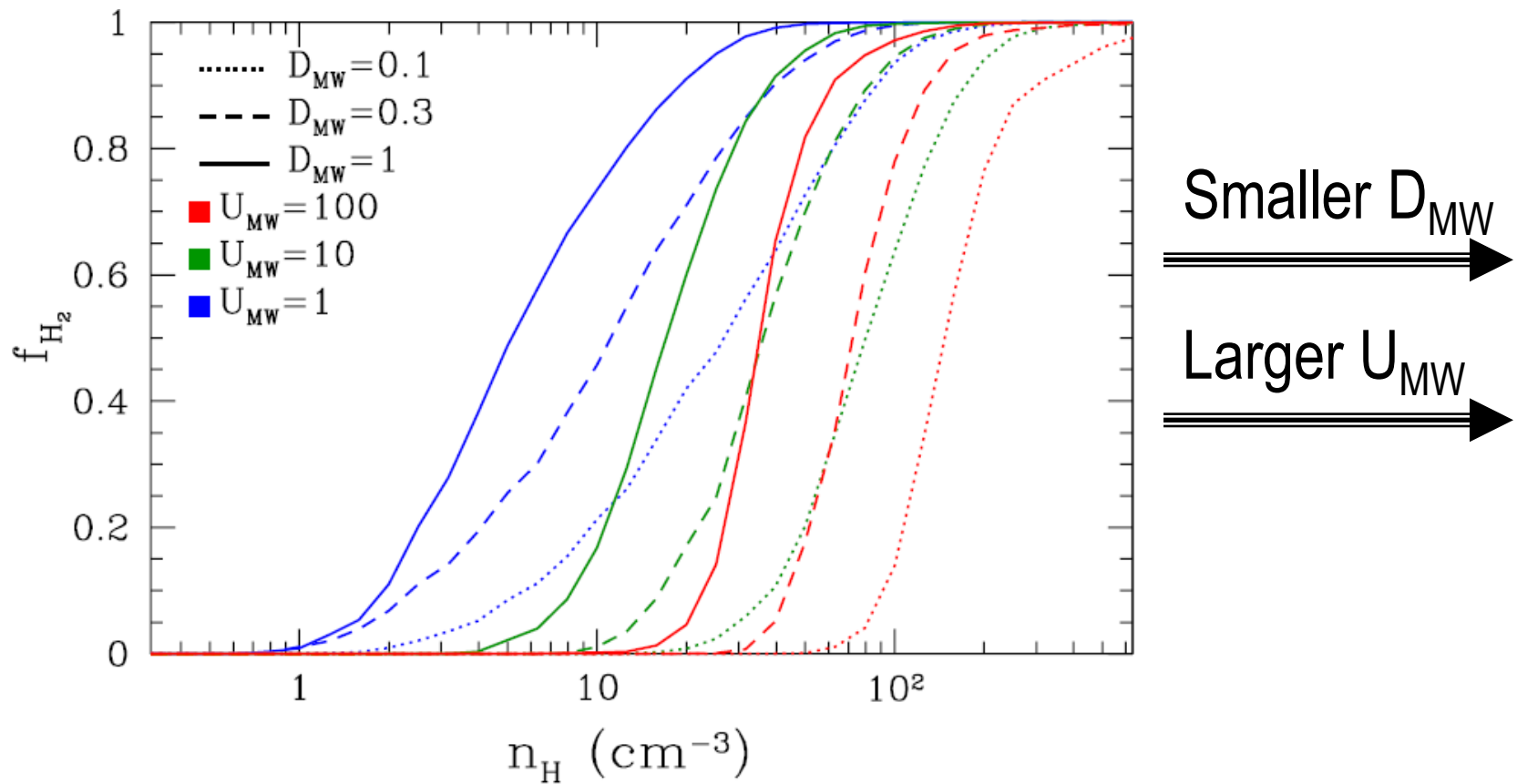
HI \rightarrow H₂ Transition: Other Galaxies

Data are from Wong & Blitz 2002



HI \rightarrow H₂ Transition: Environmental Dependence

- Transition between atomic and molecular phases scales non-trivially with the dust-to-gas ratio D_{MW} and the interstellar radiation field U_{MW} .



HI \rightarrow H₂ Transition: Numerics

- One thing we skipped over is how to define N_{H} in the code without actually doing ray tracing (of course, if you can afford ray-tracing, use ray-tracing!).
- GK11 suggested using the “Sobolev-like” approximation

$$N_{\text{H}} \equiv n_{\text{H}} L_{\text{sob}}$$

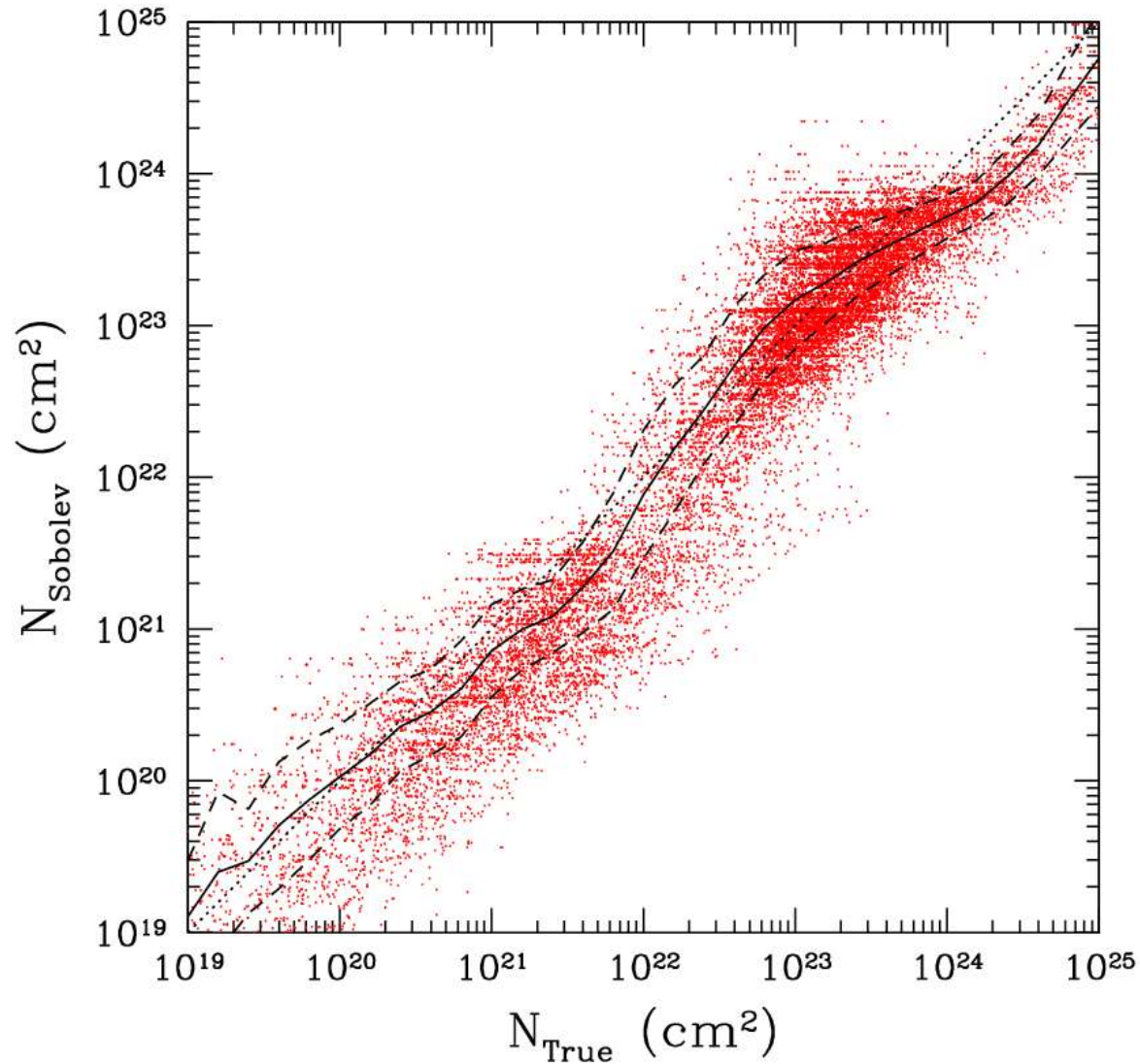
with

$$L_{\text{sob}} = C \frac{\rho}{|\nabla \rho|}$$

and C needs to be calibrated from ray-tracing.

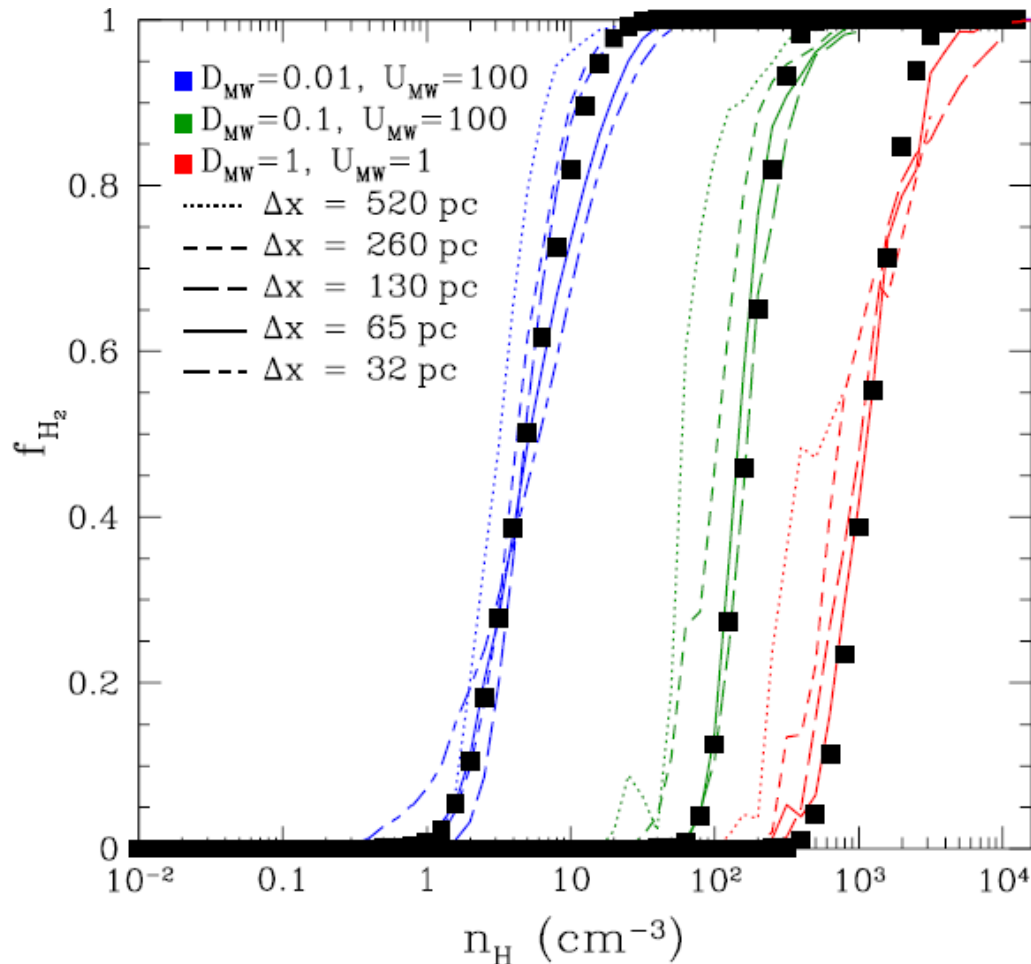
HI \rightarrow H₂ Transition: Numerics

- From calibration:
 $C \approx 0.5$.



HI \rightarrow H₂ Transition: Numerics

- What we gain from “Sobolev-like” approximation: weak resolution dependence.



- Bad idea:

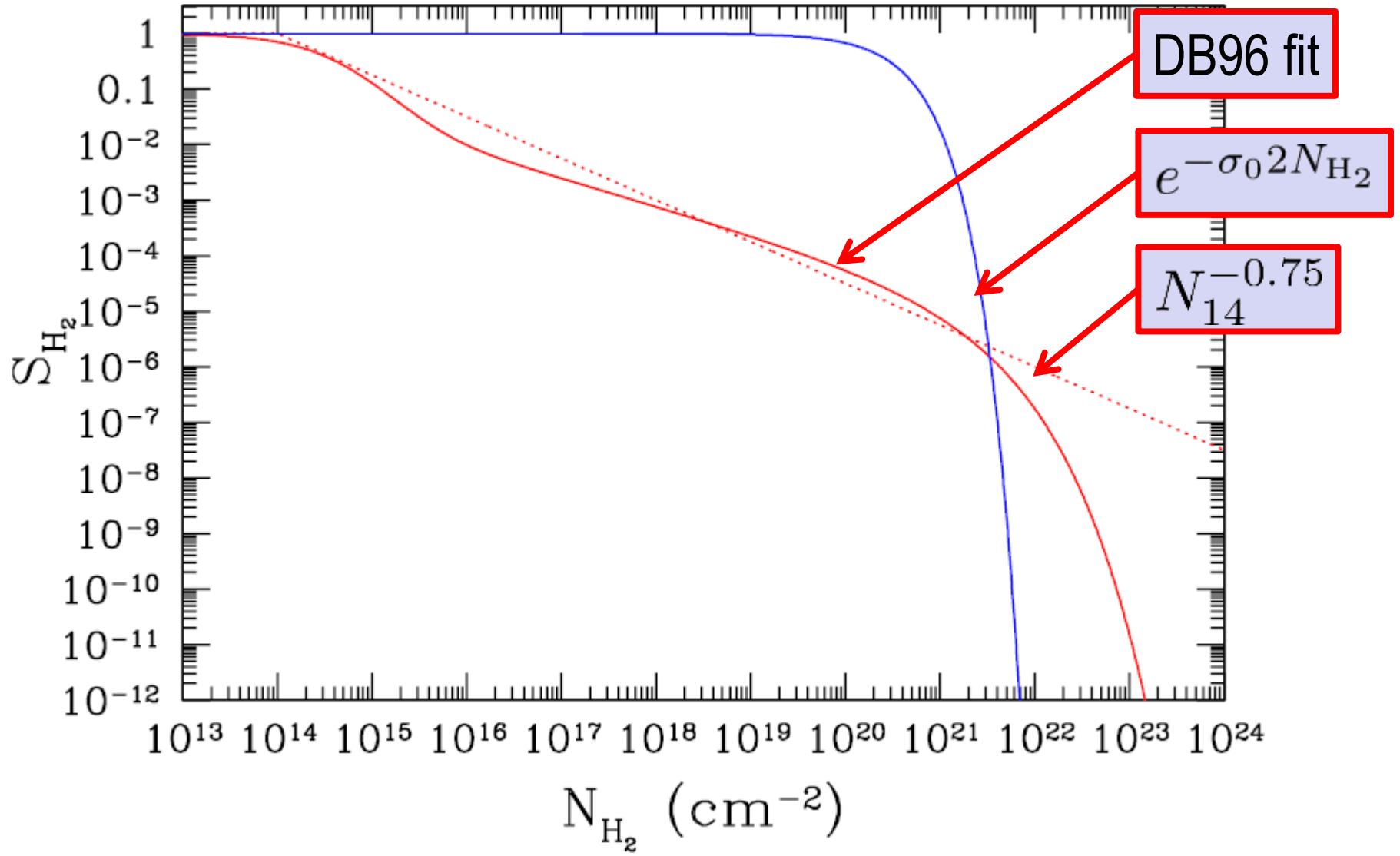
$$N_H \equiv n_H \Delta x$$

introduces explicit dependence on the cell size, say bye-bye to any hope of numerical convergence.

HI \rightarrow H₂ Transition: Parameterizations

- There are two separate parameterizations for H₂ abundance as a function of some other properties:
 1. Krumholz, McKee, & Tumlinson 2009 (KMT09) – analytical model
 - a) a “full” model as a function of U_{MW} , D_{MW} , etc
 - b) a “lite” model assuming $U_{\text{MW}} = U_{\text{MW}}(n_{\text{H}}, Z)$ $\chi \approx 3.1 \left(\frac{1 + 3.1 Z^{0.365}}{4.1} \right)$
 2. Gnedin & Kravtsov 2011 (GK11) – fits from full 3D cosmological simulations.
- But: (1a) is very similar to (2), and (1b) may work too...

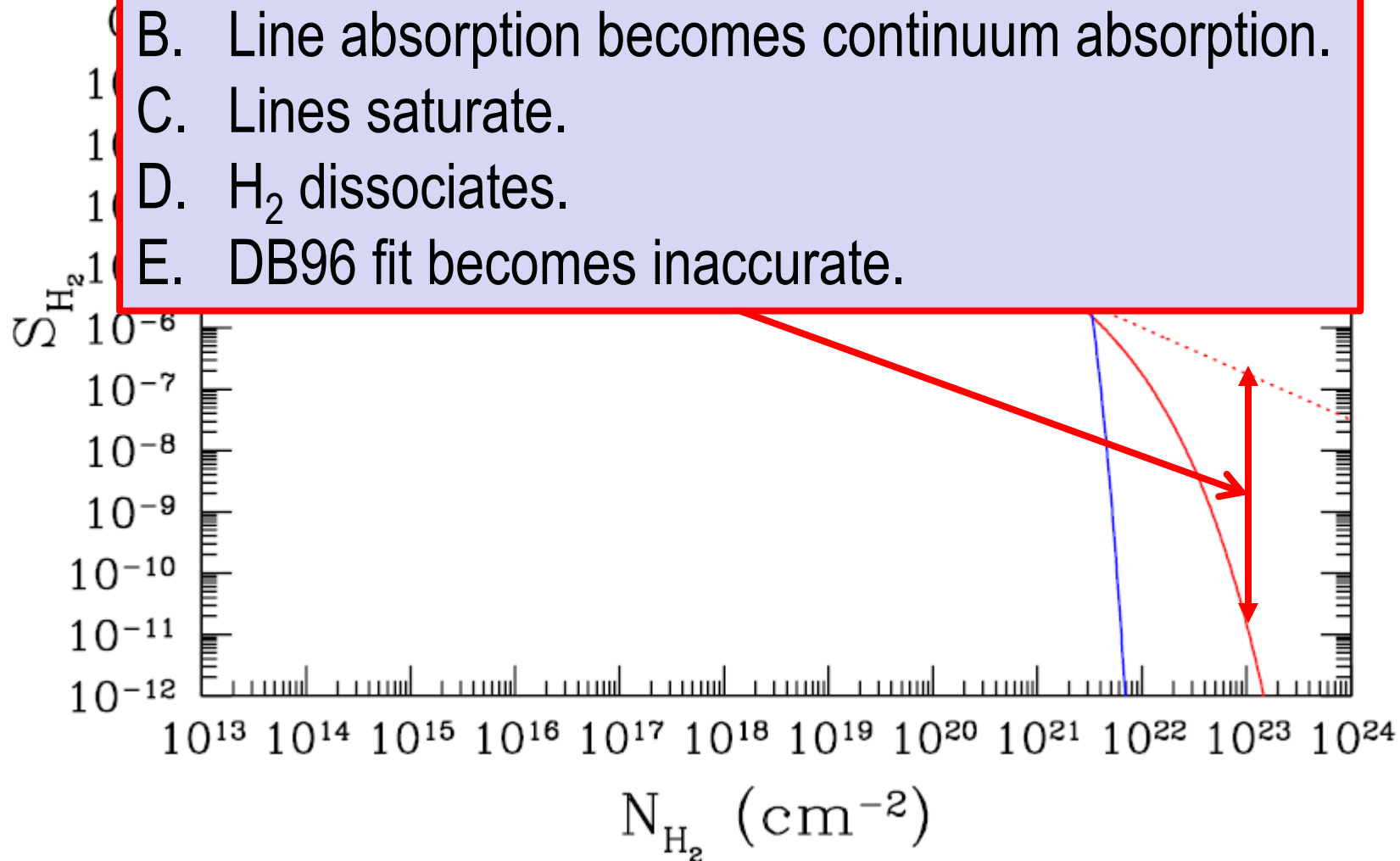
DB96 Are Back (On Feb 26, 2013)



Quiz:

What is going on there?

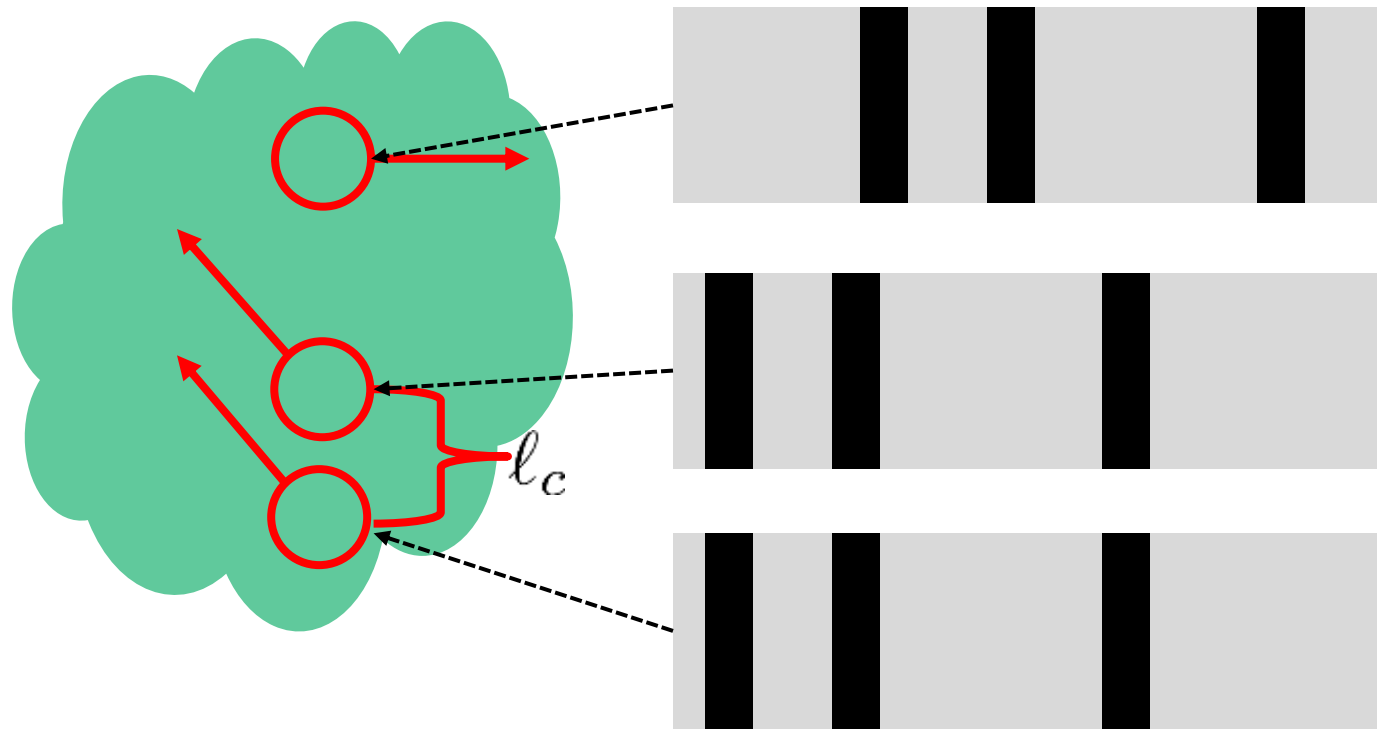
- A. Angular momentum is conserved.
- B. Line absorption becomes continuum absorption.
- C. Lines saturate.
- D. H_2 dissociates.
- E. DB96 fit becomes inaccurate.



H₂ Chemistry 101

Line Overlap

- At high enough column density H₂ lines begin to overlap...



- ...and line absorption becomes (almost) continuum absorption.

H₂ Chemistry 101

DB96+, version 2

- Once the line overlap sets in, the whole cloud starts to self-shield, i.e. $N_{\text{H}_2} \rightarrow n_{\text{H}_2} L$ (and $L \gg \ell_c$):

$$S_{\text{H}_2} = \frac{0.965}{(1 + x_1/b_5)^\alpha} + \frac{0.035}{\sqrt{1 + x_1}} e^{-0.00085\sqrt{1+x_2}}$$

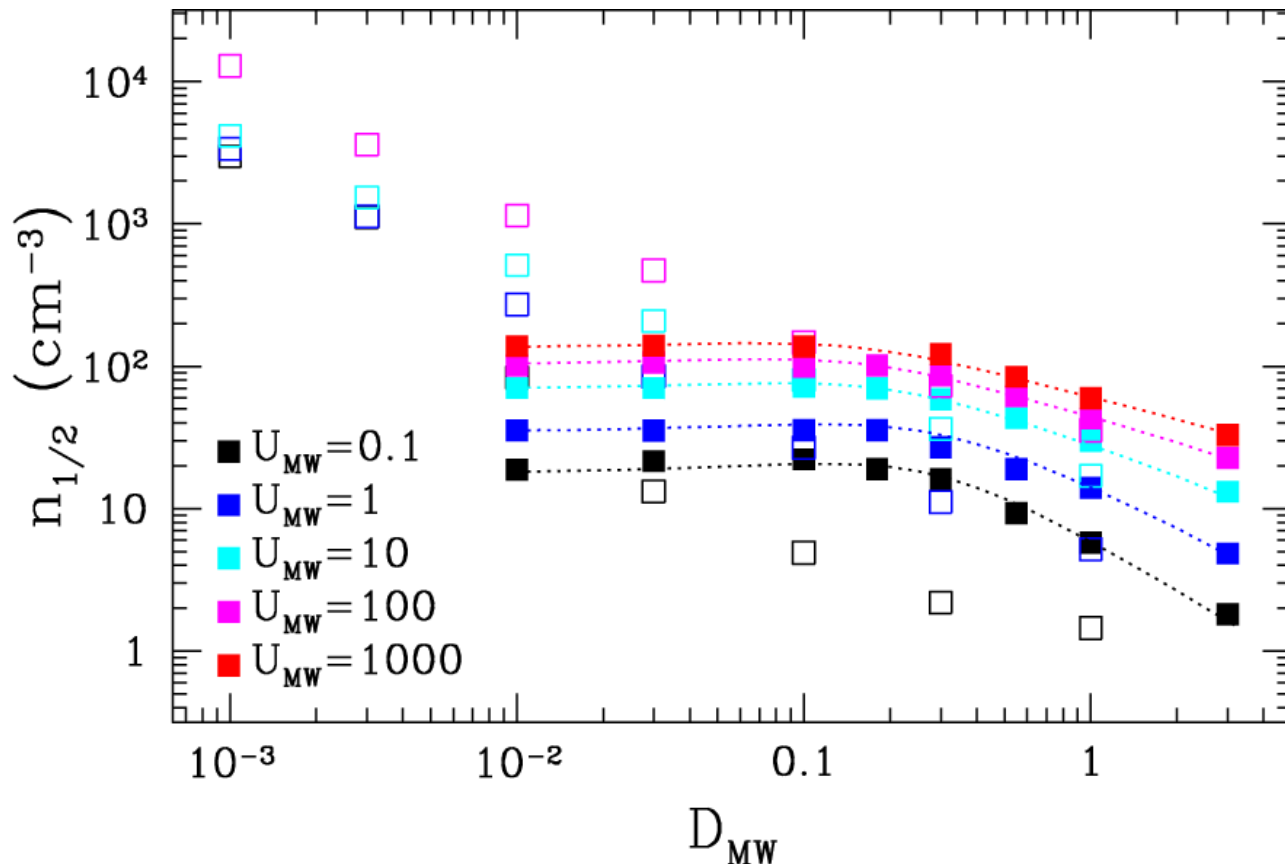
$$x_1 = \frac{n_{\text{H}_2} \ell_c}{5 \times 10^{14} \text{cm}^{-2}}$$

$$x_2 = \frac{n_{\text{H}_2} L}{5 \times 10^{14} \text{cm}^{-2}}$$

H₂ Chemistry 101

Line Overlap

- Self-shielding with line overlap dominates over dust absorption below $D_{MW} \sim 0.2$.

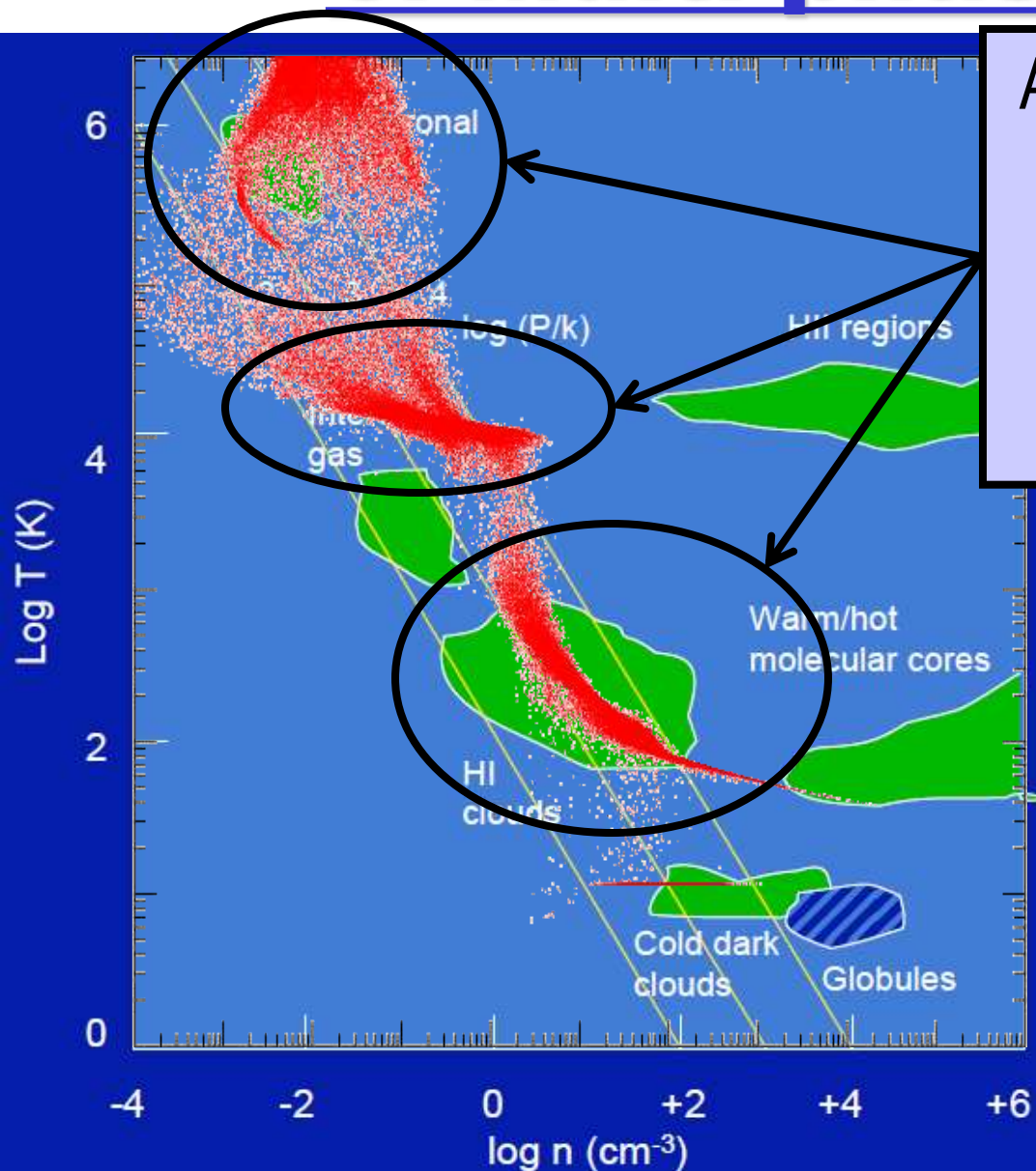


HI \rightarrow H₂ Transition, v 2.0

- As of Feb 26, 2013 neither KMT09 nor GK11 formulas are valid.
- A simple *temporary* fix is to use these approximations with $D_{MW,eff} = \max(D_{MW}, 0.2)$.
- A revised approximation is coming soon...
- **A terrific PhD project** is to take turbulent GMC simulations and post-process them with the full line RT in the LW band, testing the whole theory of the HI \rightarrow H₂ transition (dust abundance and RF dependence, line overlap, etc).



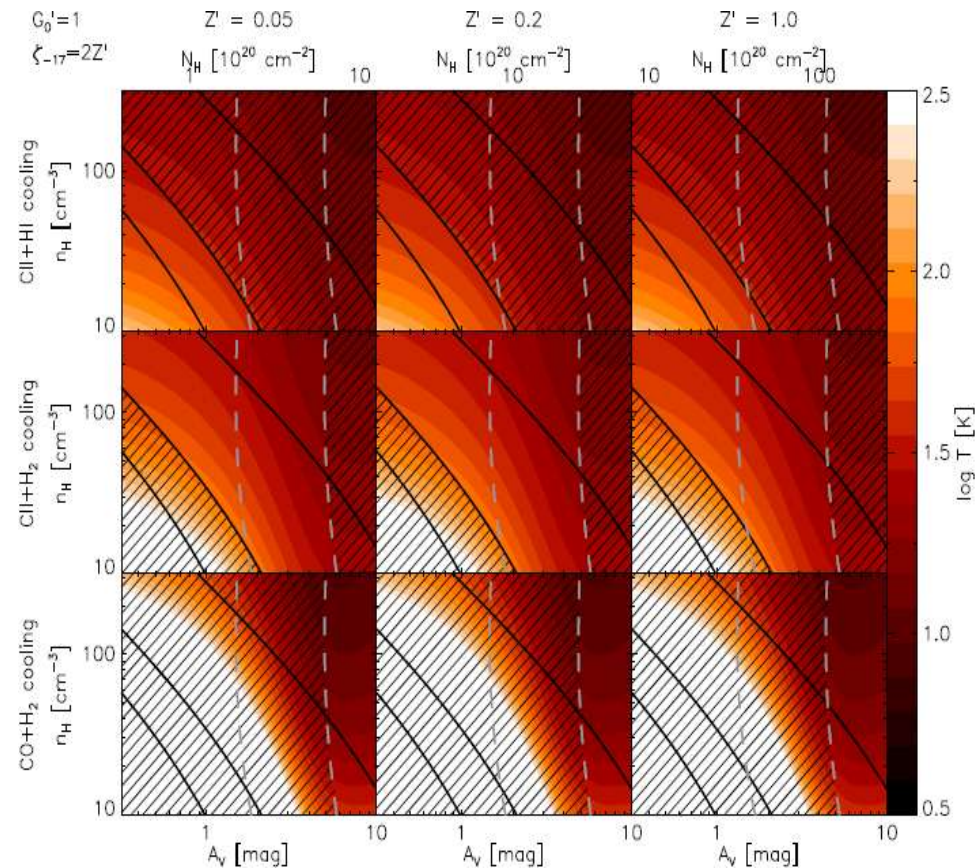
6. Multi-phase ISM



All 3 main ISM phases are there:
hot coronal gas
warm diffuse gas
cold molecular gas

Lucky “Coincidence”

- As atomic gas becomes molecular, it also becomes cold. Molecular cooling is not important – the crucial fact is shielding.
- Shielding is needed for H_2 formation; it is also needed for suppressing heating.
- The bottom line: molecular gas is always cold ($<30K$).



(Krumholz, Leroy, McKee 2011ApJ...731...25K)

Lucky “Coincidence”

- **Corollary 1:** Molecular clouds must be turbulent and turbulence must be supersonic (hence, short-lived or constantly driven).
- **Corollary 2:** Turbulence in WNM is subsonic or near-sonic (hence long-lived).
- **Corollary 3:** There cannot be large amounts of Cold Neutral Medium (CNM) – there are some observational claims to the opposite. Either those claims are wrong or we miss some fundamental ISM physics.



7. Thermodynamics of H₂

- H₂ is a diatomic molecule, its thermodynamics can be solved exactly.
- **Ideal gas quiz:** which of the following is wrong:
 - A. Adiabatic index $\gamma = c_P/c_V$.
 - B. $c_P = c_V + 1$.
 - C. For monoatomic gas $c_V = 3/2$ ($\gamma = 5/3$).
 - D. For diatomic gas $c_V = 5/2$ ($\gamma = 7/5$).

Refresher:

Statistical Mechanics of H₂

- Partition function for a diatomic molecule:

$$Z = e^{-E_n/T} Z_{\text{rot}} Z_{\text{vib}}$$

$$Z_{\text{vib}} = \sum_{v=0}^{\infty} e^{-\hbar\omega(v + 1/2)/T}$$

- The rotational part is a bit tricky, because H₂ is symmetric and two protons are indistinguishable...
- Hence, if the total spin of the nucleus is 1 (=1/2+1/2) then only odd values of $J = 1, 3, \dots$ are allowed; for zero nuclear spin (=1/2-1/2) only even $J = 0, 2, 4, \dots$ are allowed.

Refresher:

Statistical Mechanics of H₂

- $S_N = 1$: *ortho*-hydrogen molecule;
- $S_N = 0$: *para*-hydrogen molecule.

$$Z_{\text{rot}} = \frac{3}{4}Z_{\text{ortho}} + \frac{1}{4}Z_{\text{para}}$$

$$Z_{\text{ortho}} = \sum_{J=1,3,\dots} (2J + 1)e^{-\hbar^2 J(J+1)/(2IT)}$$

$$Z_{\text{para}} = \sum_{J=0,2,\dots} (2J + 1)e^{-\hbar^2 J(J+1)/(2IT)}$$

Refresher:

Statistical Mechanics of H₂

Quiz:

? *What is the partition function used for?*

- A. For partitioning.
- B. For partying.
- C. To answer all questions.
- D. To measure the thermodynamic state of the gas.

Refresher:

Statistical Mechanics of H₂

- The partition function is used to derive all other quantities:

- Free energy:
$$F = -T \log \left[\frac{V}{N!} \left(\frac{mT}{2\pi\hbar^2} \right)^{3/2} Z \right]$$

- Pressure:
$$P = - \left. \frac{\partial F}{\partial V} \right|_T$$

- Entropy:
$$S = - \left. \frac{\partial F}{\partial T} \right|_V$$

- Internal energy:
$$E = F + TS$$

Refresher:

Statistical Mechanics of H₂

- Specific heats:

$$c_V = \frac{1}{N} \left. \frac{\partial E}{\partial T} \right|_V$$

$$c_P = c_V + 1$$

- For diatomic molecule:

$$c_V = \frac{3}{2} + c_{V,\text{rot}} + c_{V,\text{vib}}$$

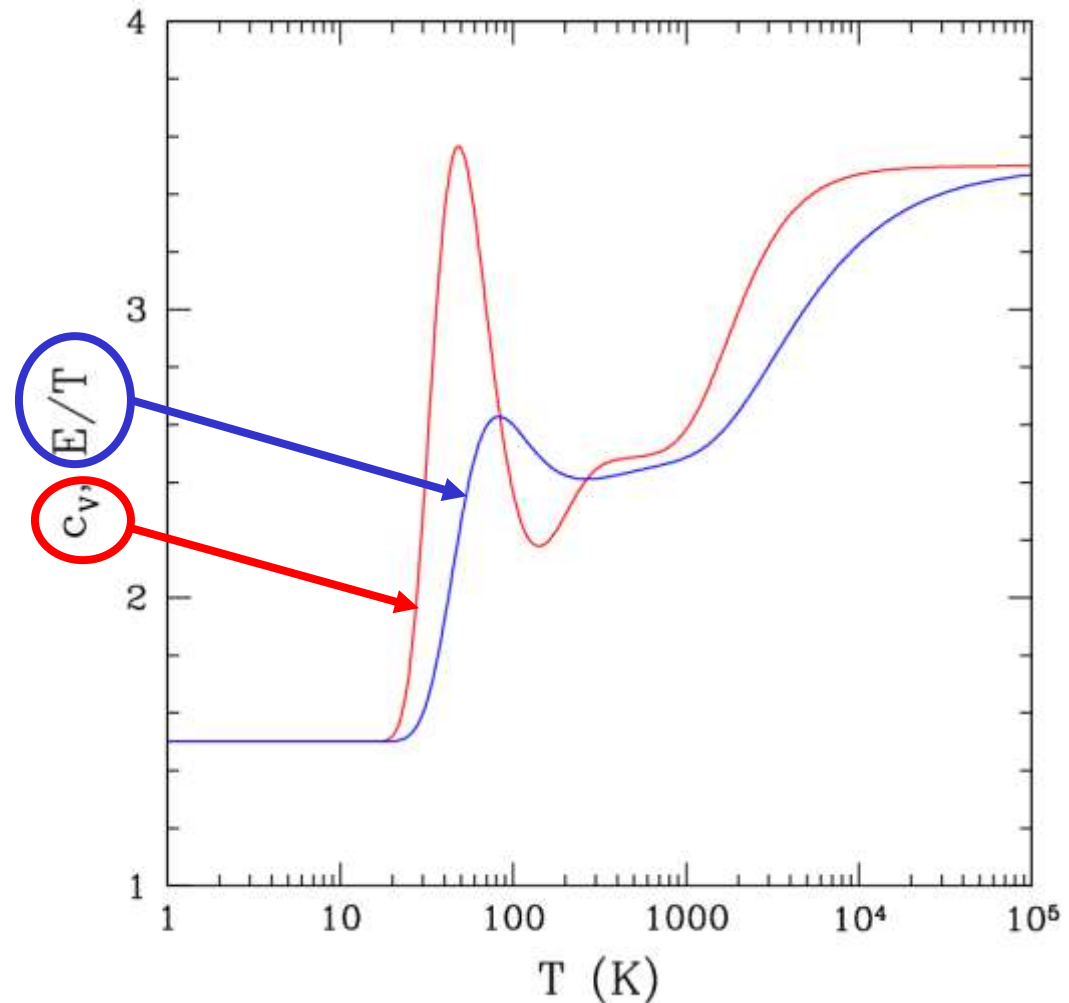
Thermodynamics of H₂

- H₂ is either not polytropic at all ($T > 20\text{K}$)

$$c_V \neq \text{const}$$
$$E \neq c_V T$$

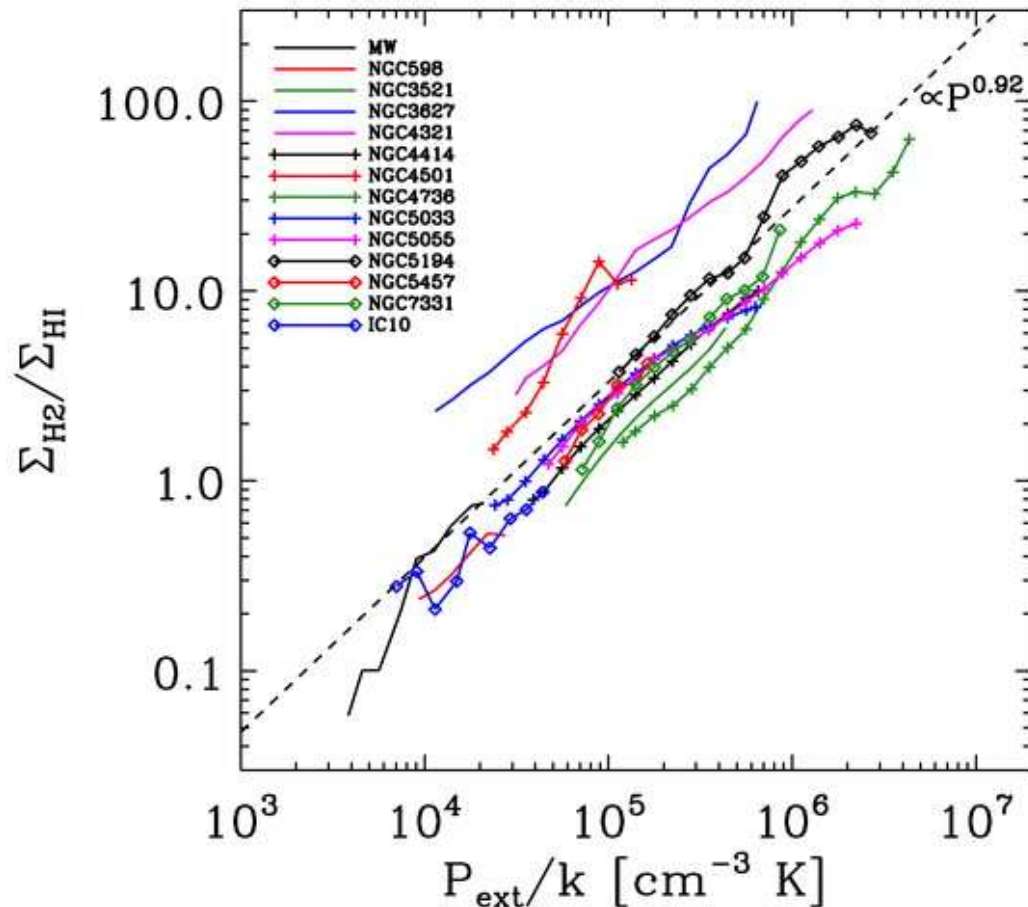
or behaves as
monoatomic gas
($T < 20\text{K}$)

$$c_V = 3/2$$
$$\gamma = 5/3$$



8. Blitz-Rosolowsky Relation

- There exist a correlation between the “external pressure” and molecular fraction on large scales.
- Discovered by Leo Blitz & Erik Rosowsky (2006ApJ...650..933B).
- The scatter around the mean relation is substantial.
- Relation defined on $\sim 1\text{kpc}$ scales.



BR Relation

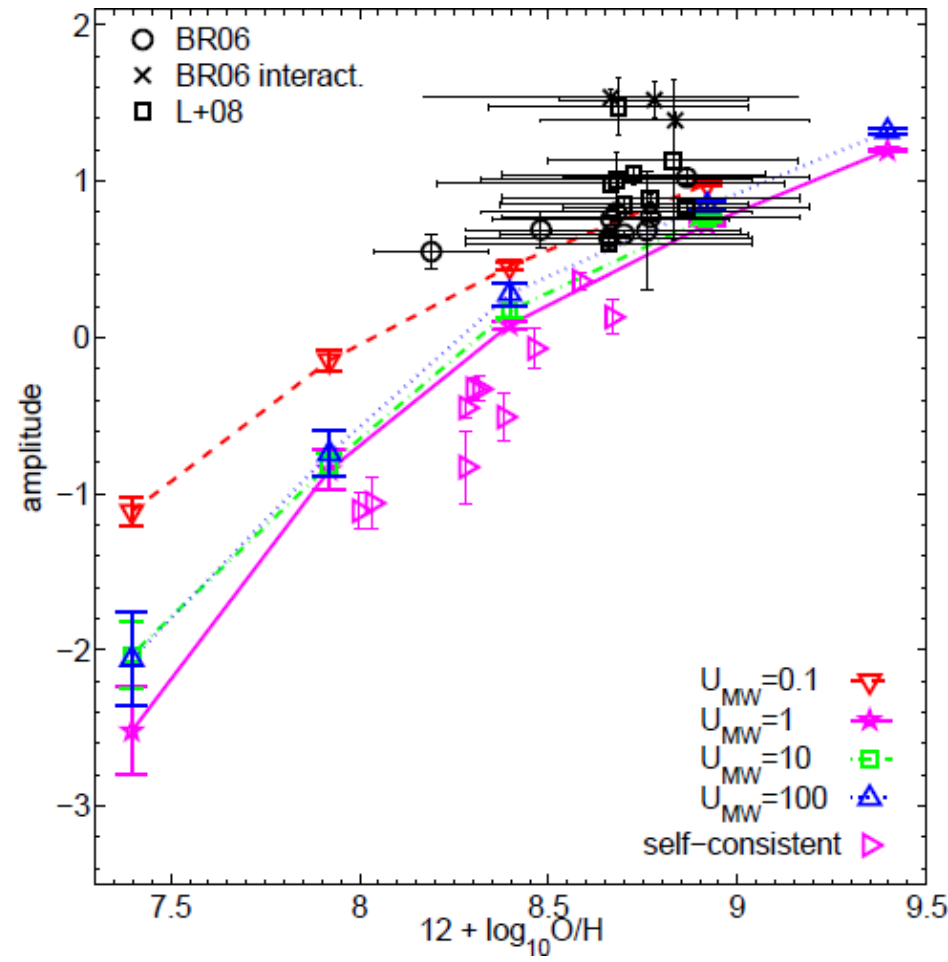
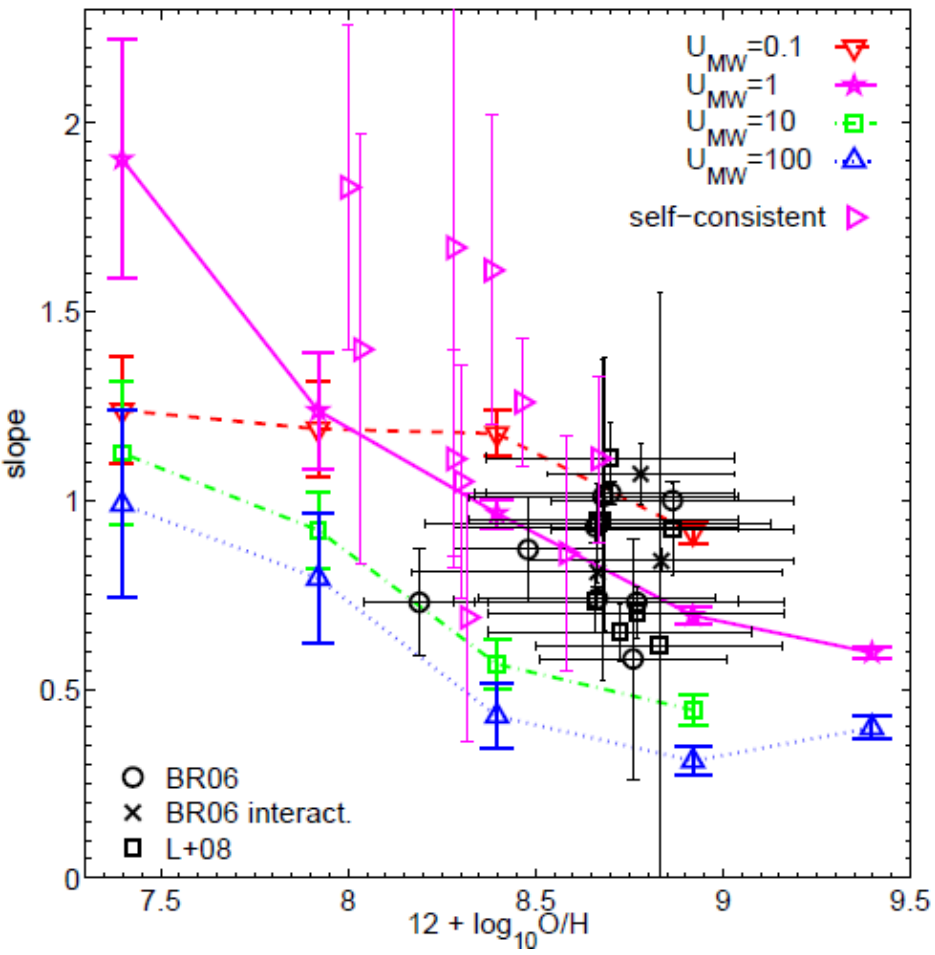
- BR06 do not actually measure pressure, they derive a proxy for it:

$$P_{\text{ext}} \approx 0.84\sqrt{G}\Sigma_g\sigma_g \left[\left(\frac{\Sigma_*}{h_*} \right)^{1/2} + \left(\frac{\pi\Sigma_g}{4h_g} \right)^{1/2} \right]$$

- σ_g , h_* , and h_g are approximately constant.
- Hence, the “external pressure” is essentially a proxy for the gas surface density and the BR relation should follow from the physics of $\text{HI} \rightarrow \text{H}_2$ transition.

BR Relation

- BR relation depends on the environment and will change with galaxy metallicity and ISRF strength.



9. Cosmic Pandora Box: The X-Factor

- Classic Catch-22: H_2 has to be shielded from the outside in the LW band.
- Hence, the “outside” (i.e. us) cannot see LW emission from molecular gas.
- On top of that, the same dust obscures background sources, making absorption spectroscopy very difficult.
- The standard way to observe molecular clouds is via their CO emission.

CO Spectrum

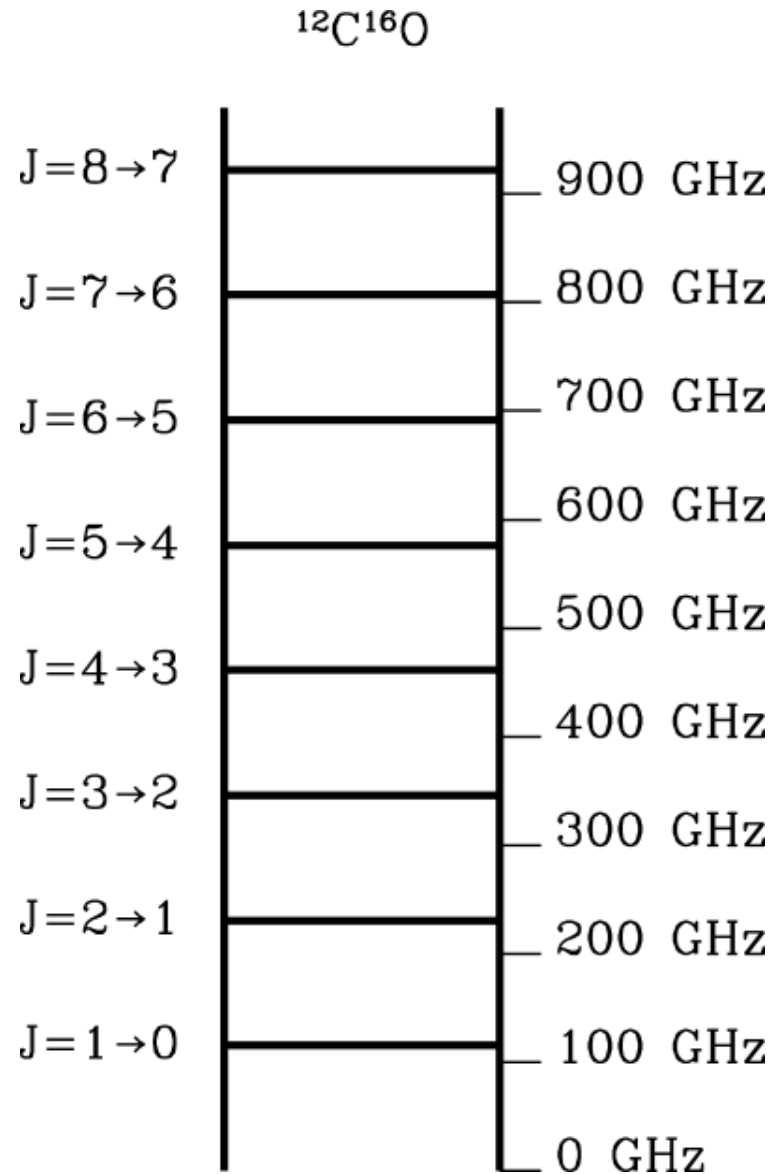
- For rotational transitions:

$$\nu_J = \frac{\hbar J}{2\pi I}$$

- For CO(1-0):

$$\nu_{1 \rightarrow 0} = 115 \text{ GHz}$$

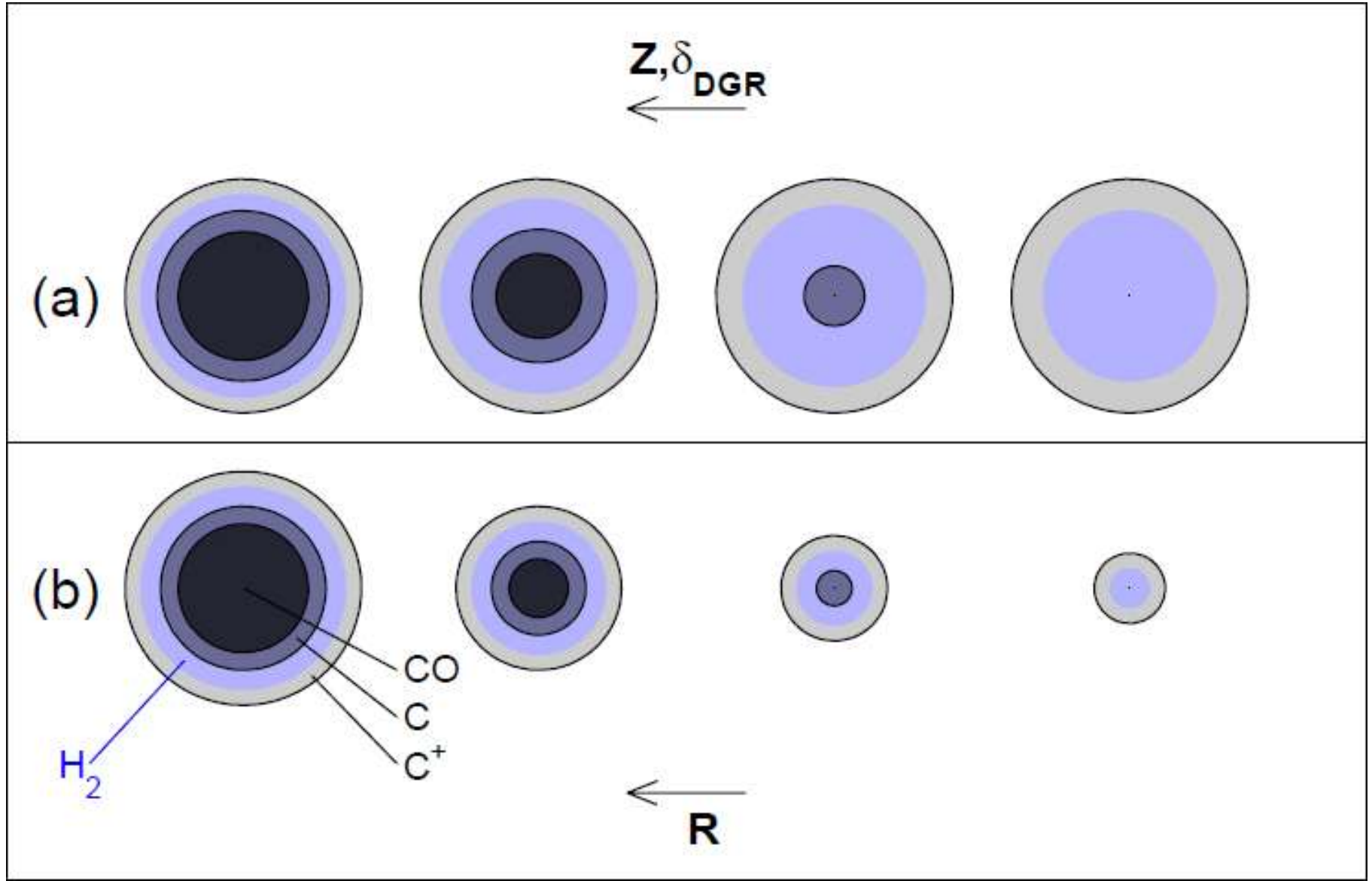
$$\lambda_{1 \rightarrow 0} = 2.6 \text{ cm}$$



CO as H₂ Tracer

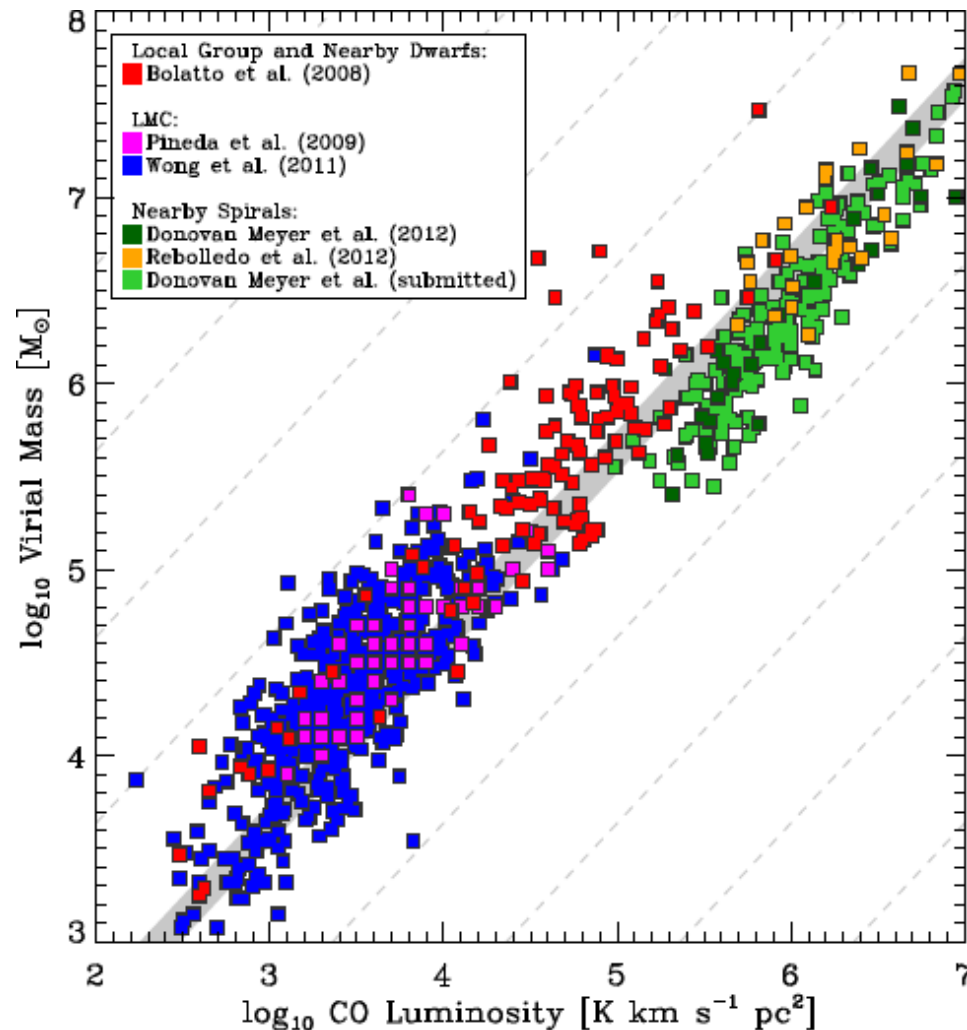
- A priori there is no reason why CO should be a good tracer of H₂:
 - CO needs higher dust shielding to form;
 - CO gets saturated at too high column densities;
- Hence, CO emission comes from a narrow range of column densities, both cloud outskirts and cloud centers emit little.

CO as H₂ Tracer



CO as H₂ Tracer

- Never-the-less, miracles do happen...
- Part of the reason for the X_{CO} miracle is that galaxies contain the whole spectrum of molecular clouds, hence averaging reduces variety.



CO as H₂ Tracer

- In galactic studies a relevant quantity is an “X-Factor”,

$$X_{\text{CO}} = \frac{N_{\text{H}_2}}{W_{\text{CO}}}$$

and W_{CO} is the line equivalent width (i.e. different for different transitions).

$$W_{\text{CO}} = \int T_A(v) dv = T_B \int \beta(v) dv$$

- The “Galactic value” is

$$X_{\text{CO}} = 2 \times 10^{20} \frac{\text{cm}^{-2}}{\text{K km/s}}$$

CO as H₂ Tracer

- In extra-galactic studies a galaxy is rarely resolved (until the full ALMA comes online), so a convenient quantity is

$$\alpha_{\text{CO}} = \frac{1.36 M_{\text{H}_2}}{L_{\text{CO}}}$$

and L_{CO} is the total CO luminosity (in the specific line being observed).

- The “Galactic value” is

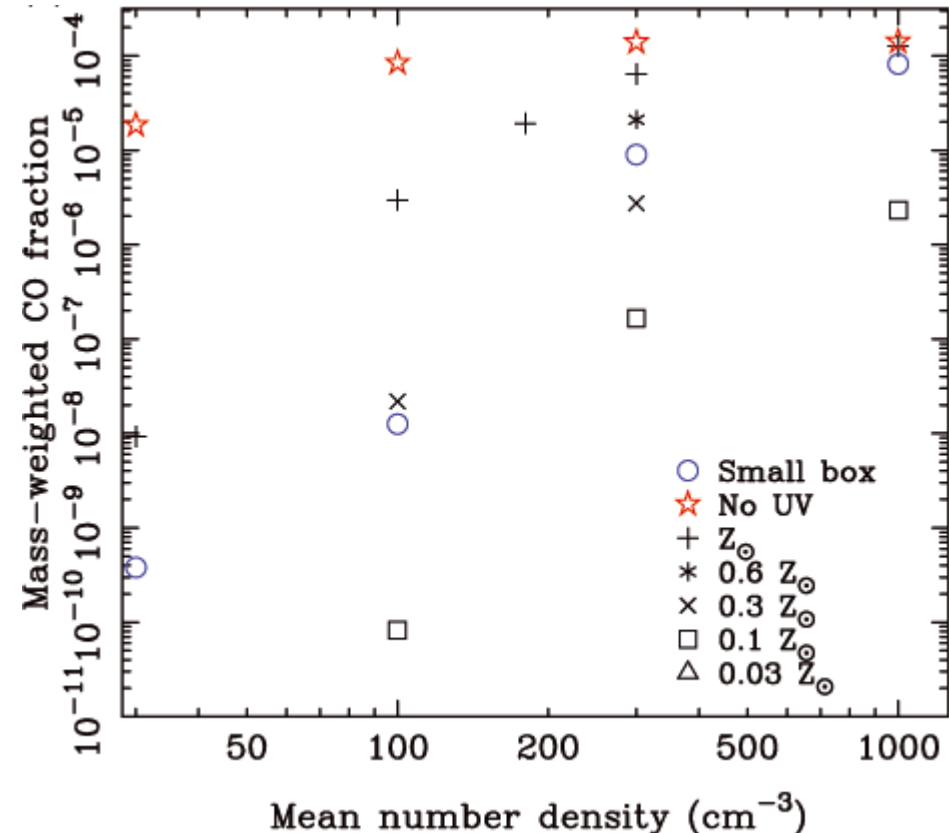
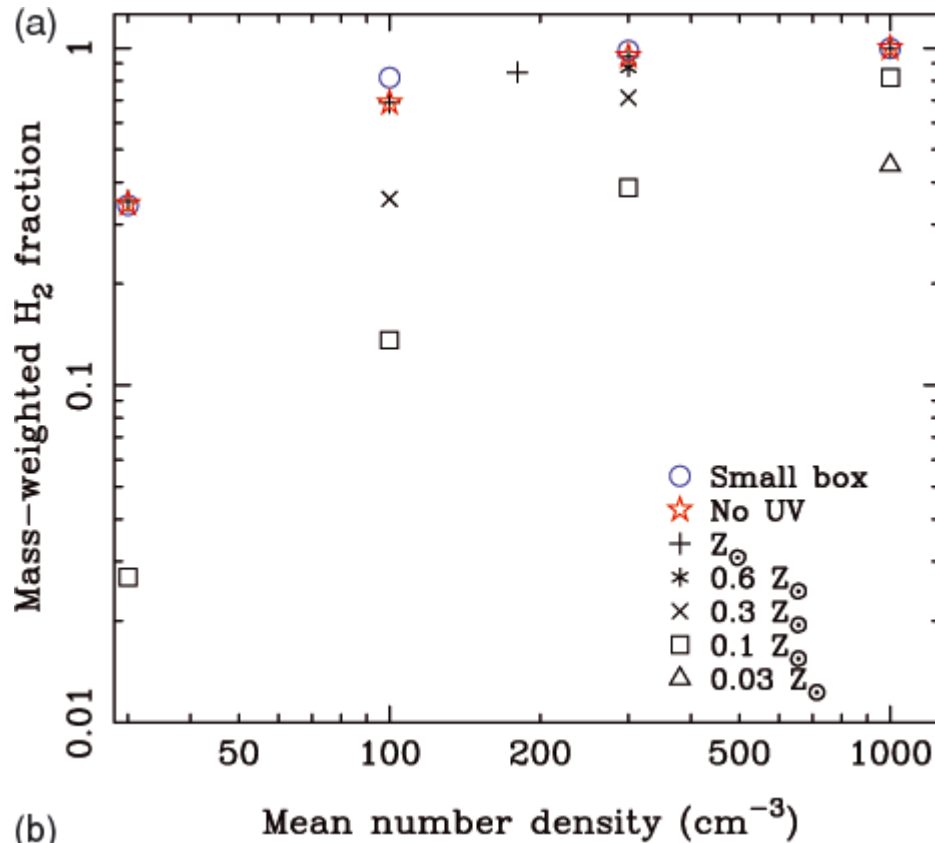
$$\alpha_{\text{CO}} = 4.3 \frac{M_{\odot}/\text{pc}^2}{\text{K km/s}}$$

Modeling CO Emission

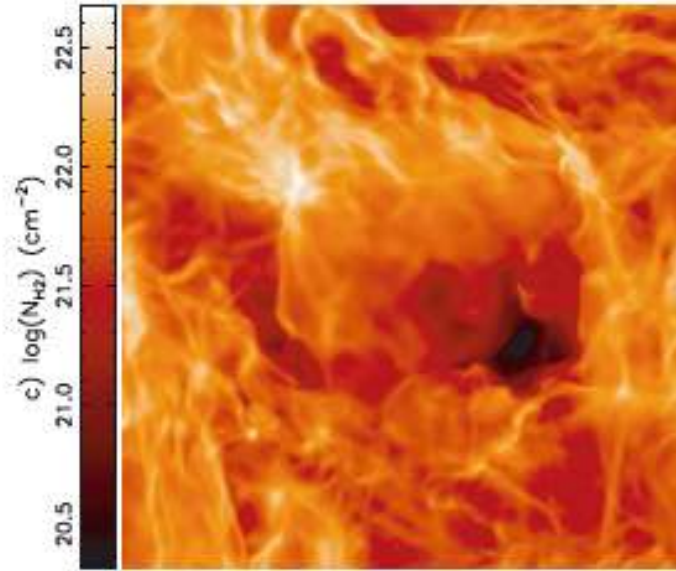
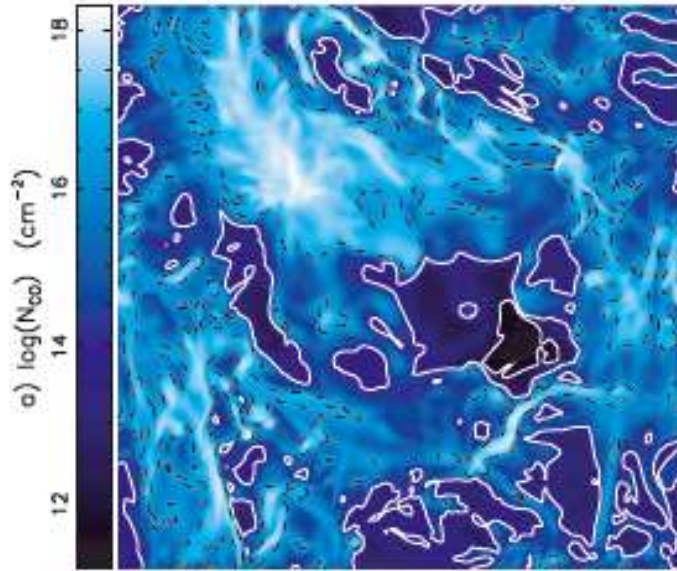
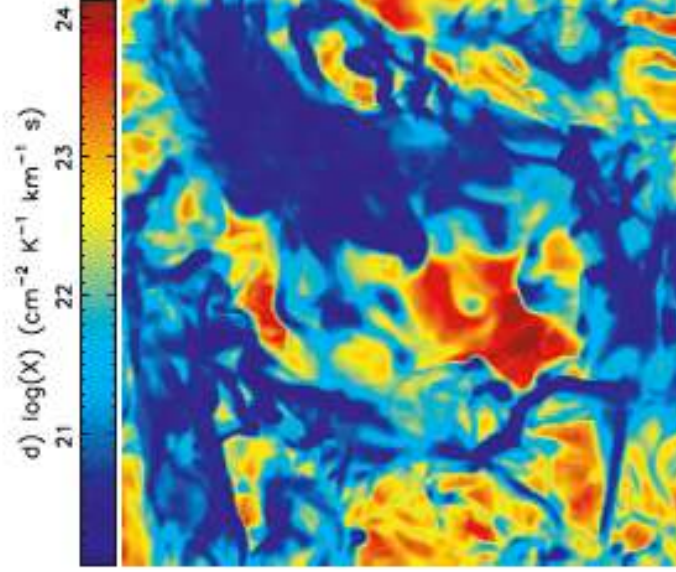
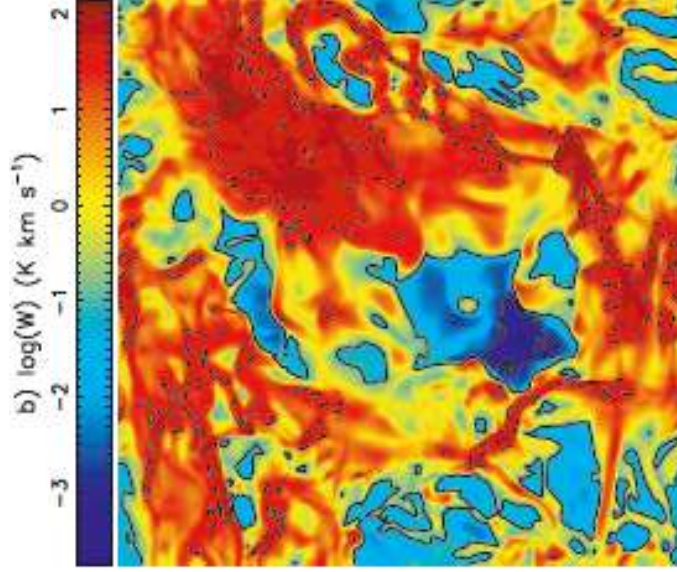
- Scales on which CO emission originates are not resolvable in modern cosmological or galactic simulations. Hence, it needs to be followed with a *sub-grid model*.
- But since it is not important dynamically, it can be modeled in *post-processing*.
- The best (in principle) sub-grid model is a someone's else simulation!

Modeling CO Emission

- Glover & MacLow (2011MNRAS.412..337G)
- 20pc box with all the physics.

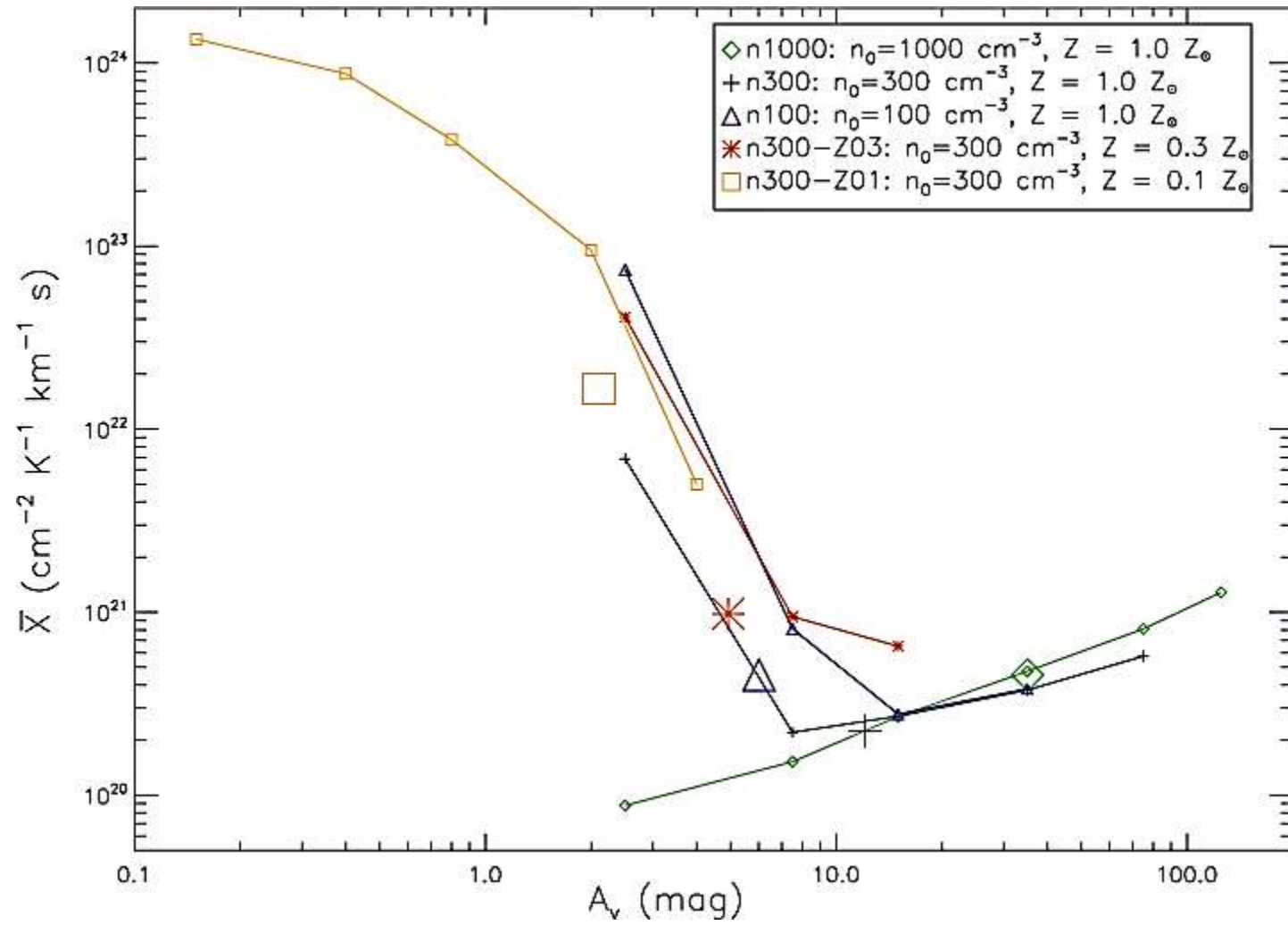


Modeling CO Emission



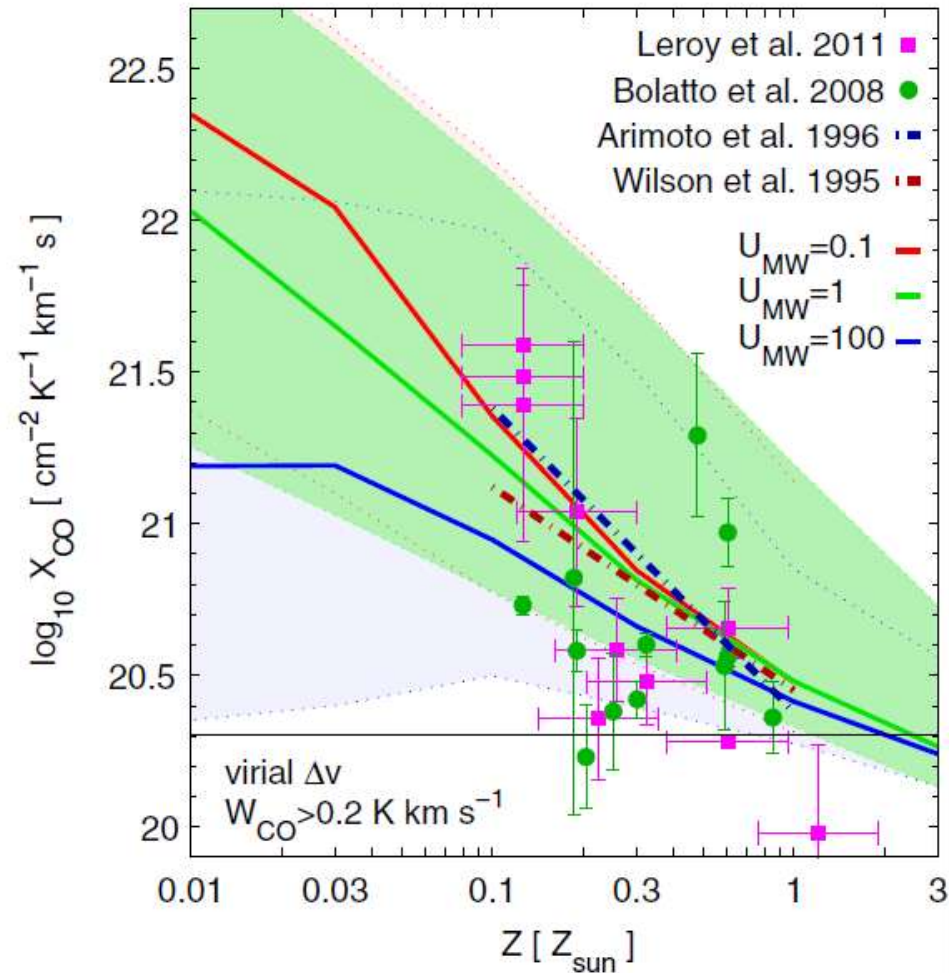
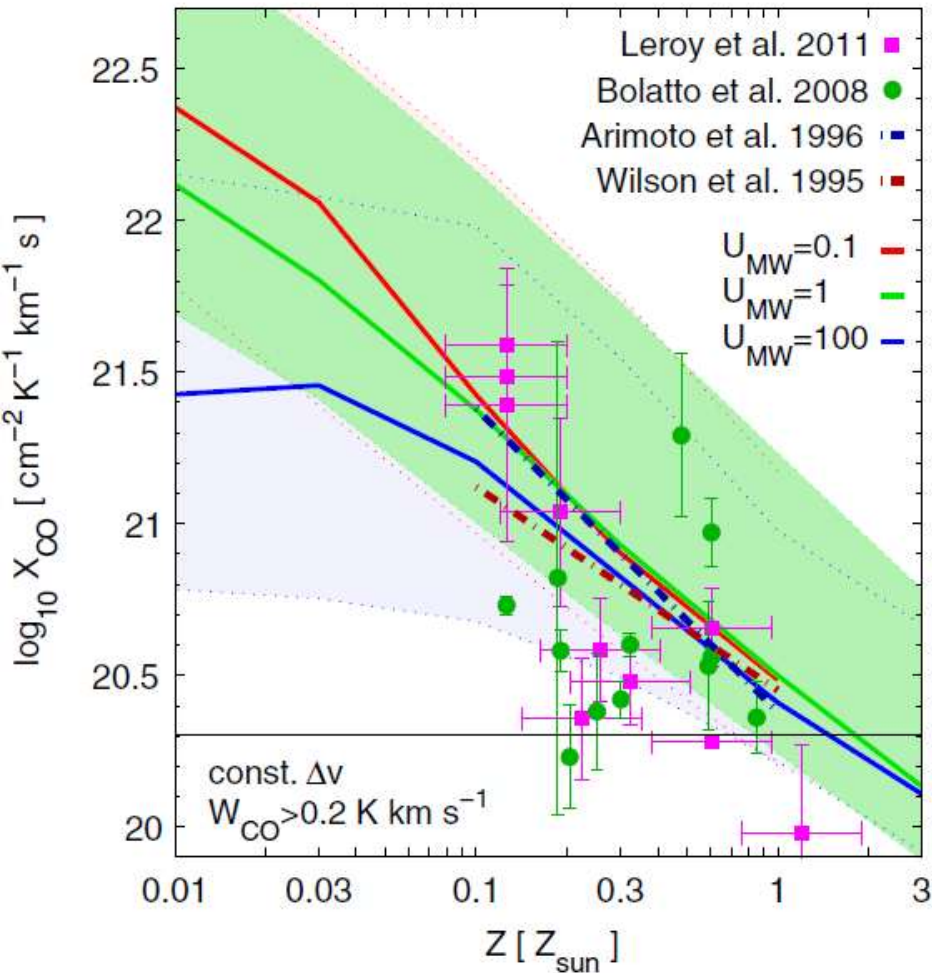
Modeling CO Emission

- X_{CO} primarily depends on A_V .



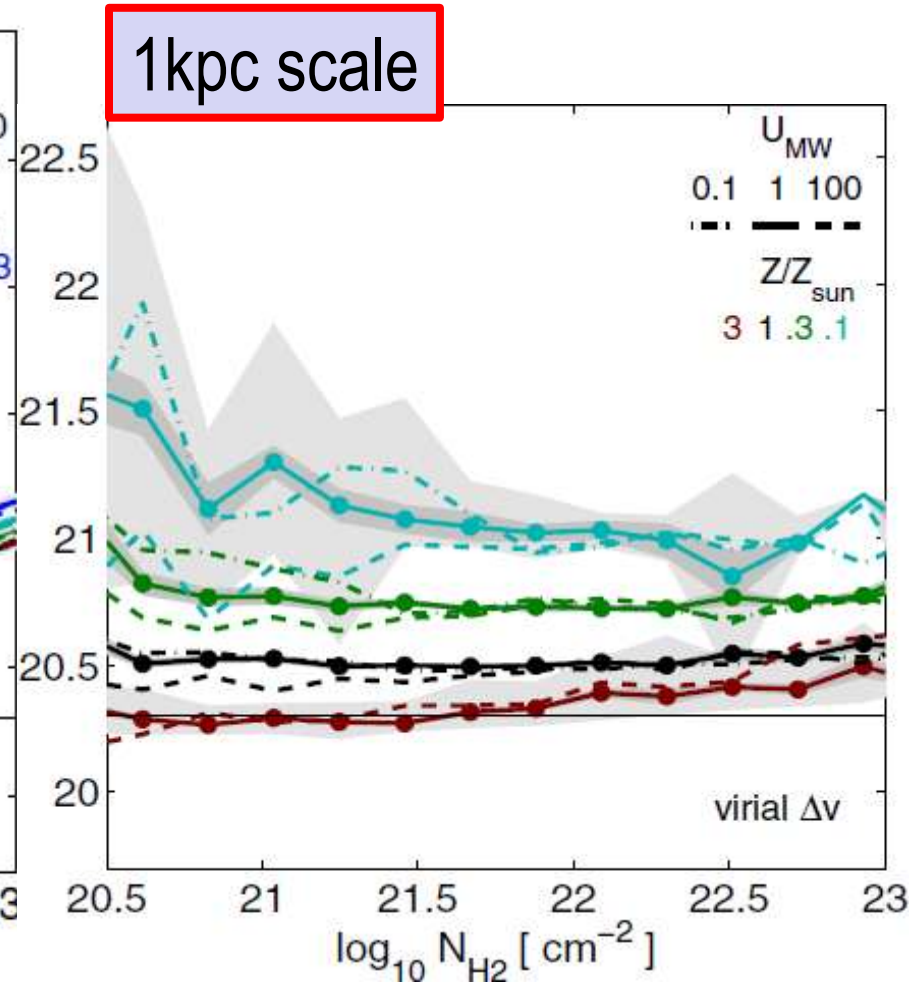
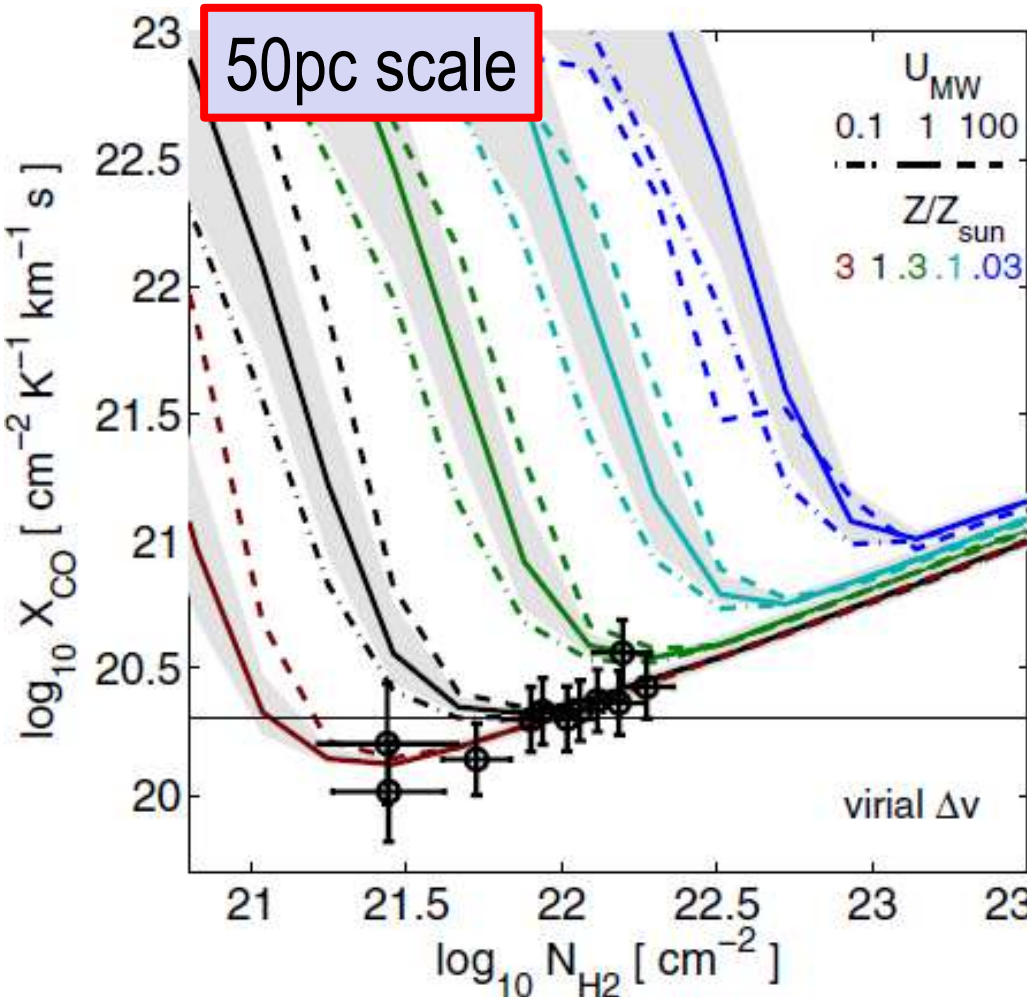
Modeling CO Emission

- Feldman, Gnedin, & Kravtsov (2012ApJ...747..124F)



Modeling CO Emission

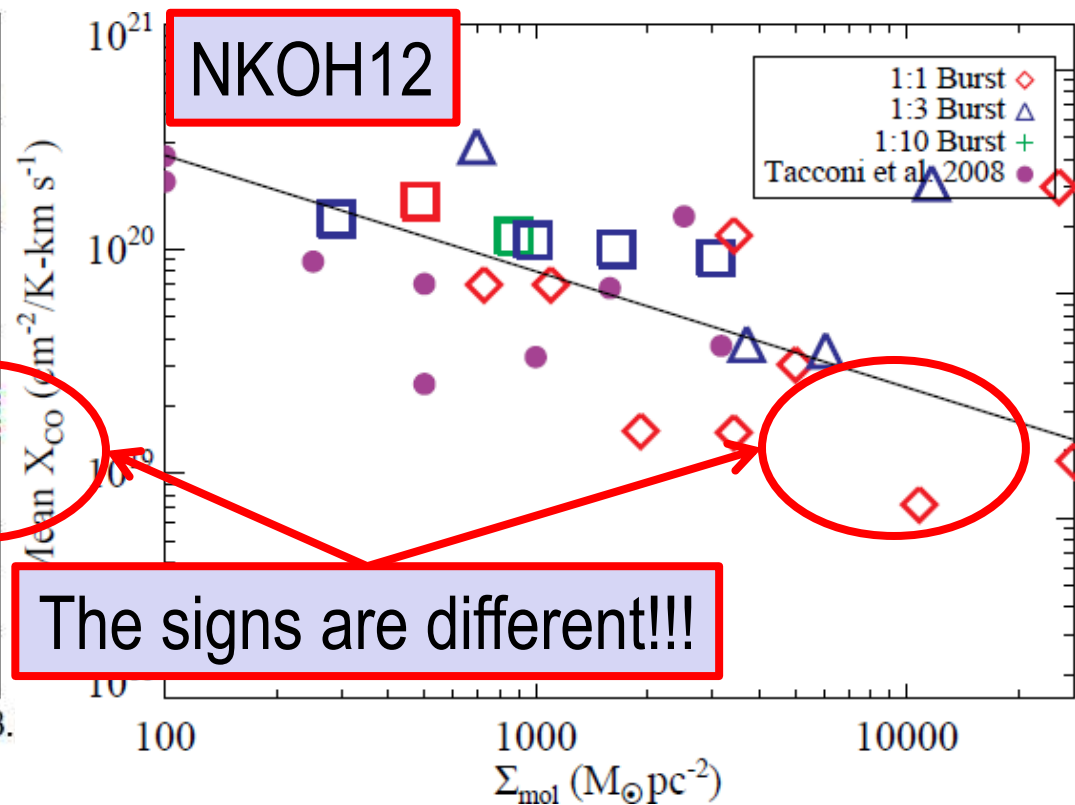
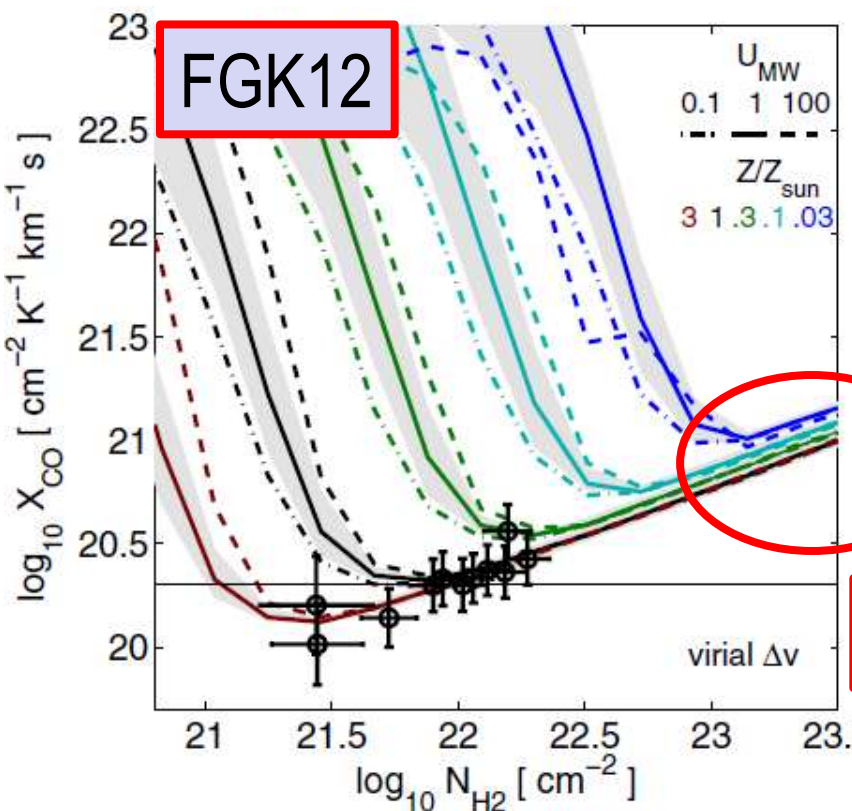
- The power of averaging: most of N_{H_2} variation goes away.





Modeling CO Emission: A Word of Caution

- Alternative X_{CO} model: Narayanan et al (2012MNRAS.421.312).



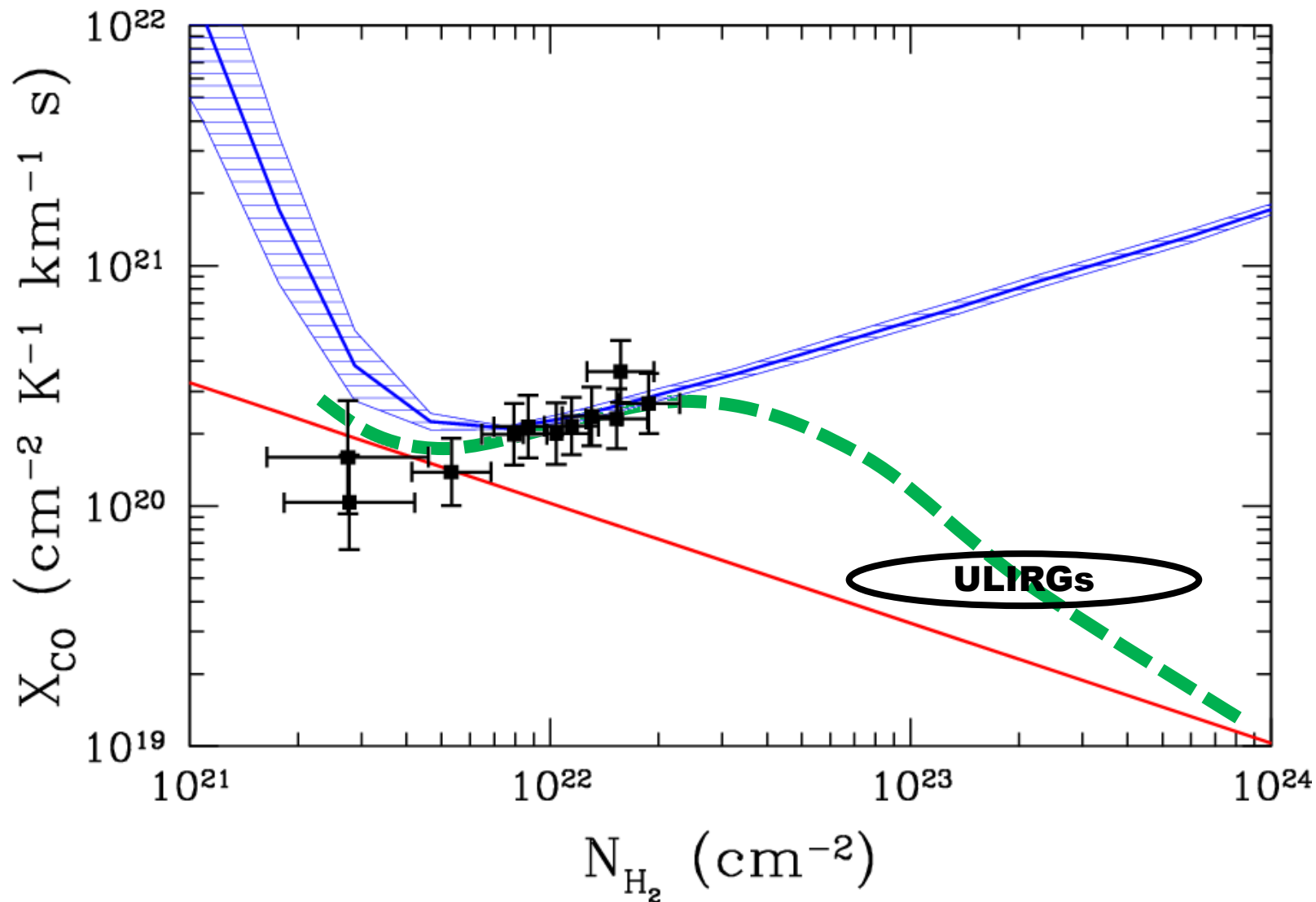
Modeling CO Emission: Pros and Cons



	FGK12	NKOH12
• Based on ISM-scale simulations	<input checked="" type="checkbox"/>	<input type="checkbox"/>
• Accounts for radiation field	<input checked="" type="checkbox"/>	<input type="checkbox"/>
• Accounts for dust-to-gas coupling	<input type="checkbox"/>	<input checked="" type="checkbox"/>
• FGK12 and NKOH12 models should be taken as upper and lower limits respectively.		
• The truth is probably somewhere in between, still waiting to be discovered...		



Modeling CO Emission: Truth is Left for the Future



10. Cosmic Pandora² Box: The X-Factor in ULIRGS and ODPs*

- X_{CO} factor depends inversely on the line brightness temperature:

$$X_{\text{CO}} = \frac{N_{\text{H}_2}}{T_B \Delta v}$$

- Most molecular clouds in the MW and other normal galaxies have $T \approx 10\text{K}$, but cosmic dust is usually warmer, $T_{\text{dust}} = 40 - 60\text{K}$. Hence, if dust and gas couple, T_B can go up.

* Other Dense Places

ULIRGs

- The box was opened by Solomon, Downes, Radford, and Barrett (1997ApJ...478..144S):

$$\frac{M_{\text{dyn}}(\text{core})}{L'_{\text{CO}}} = \frac{M_{\text{dyn}}(\text{min})}{L'_{\text{CO}}} \left(\frac{1}{f_V}\right)^{0.5} \left(\frac{L'_{\text{core}}}{L}\right)^{0.5} \left[\frac{T_{\text{bb}}}{T_b(\text{CO})}\right]^{0.5} . \quad (17)$$

For the values suggested above, namely, $f_V = 0.5$, $(L'_{\text{core}}/L) = 0.5$, and $T_{\text{bb}}/T_b(\text{CO}) = 2$, the true dynamical mass and the ratio M_{dyn}/L would both be $2^{1/2}$ times higher than the values in Table 3.

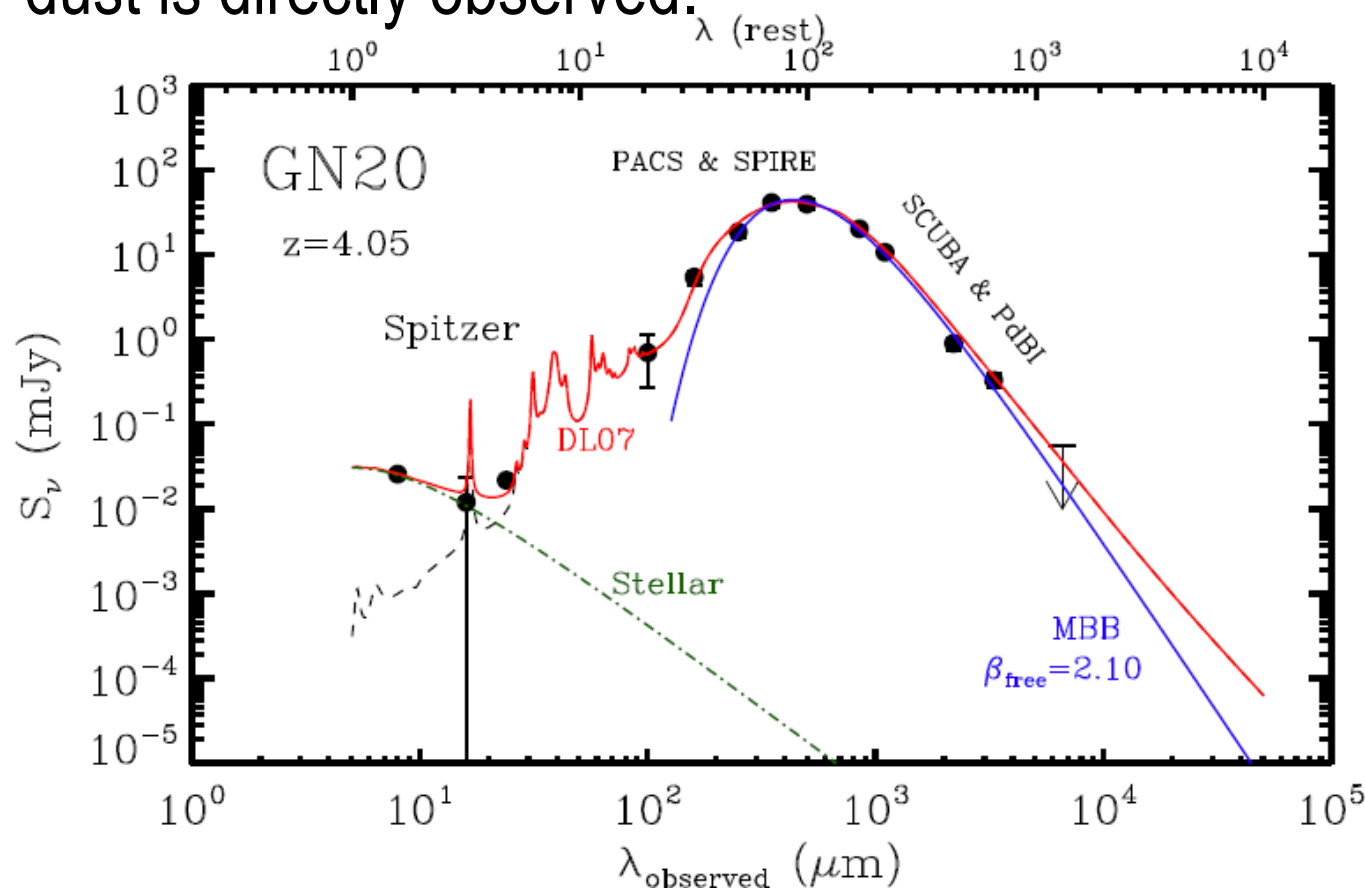
- This result is often mis-interpreted: $\alpha_{\text{CO},\text{min}}$ is taken as the actual value for α_{CO} , biasing the conclusions.



Herschel's Legacy

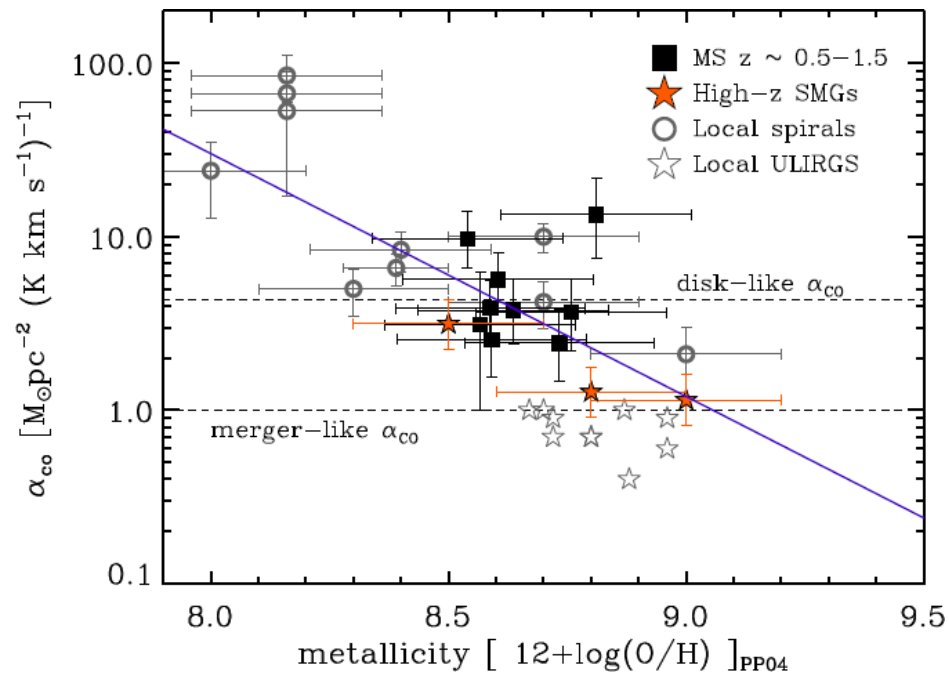
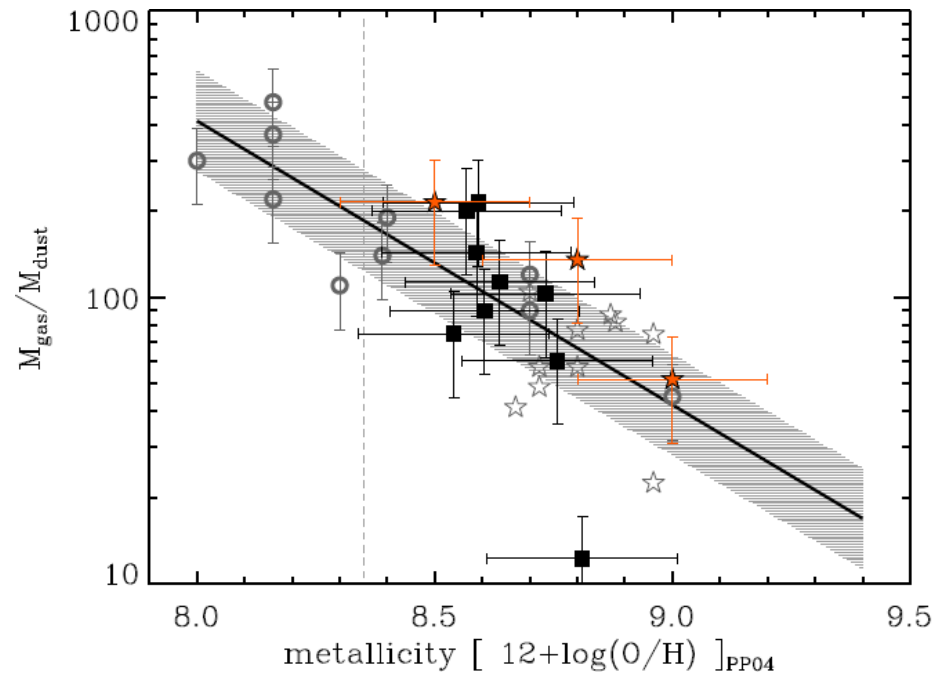


- With Herschel, this question can now be resolved, since the dust is directly observed.



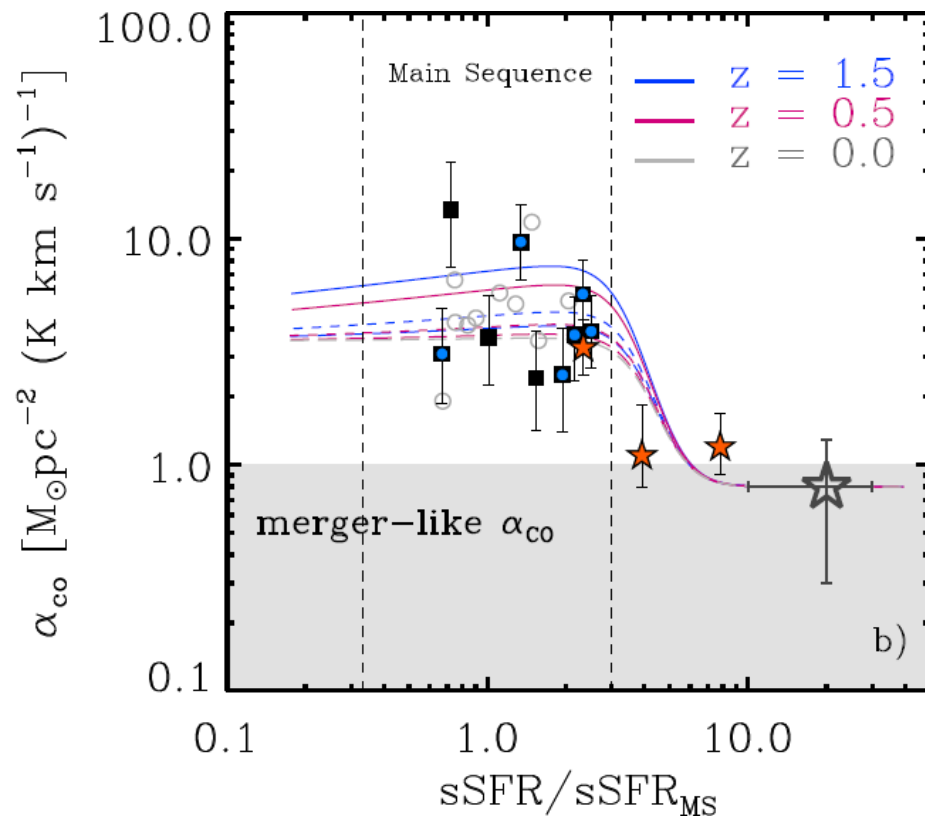
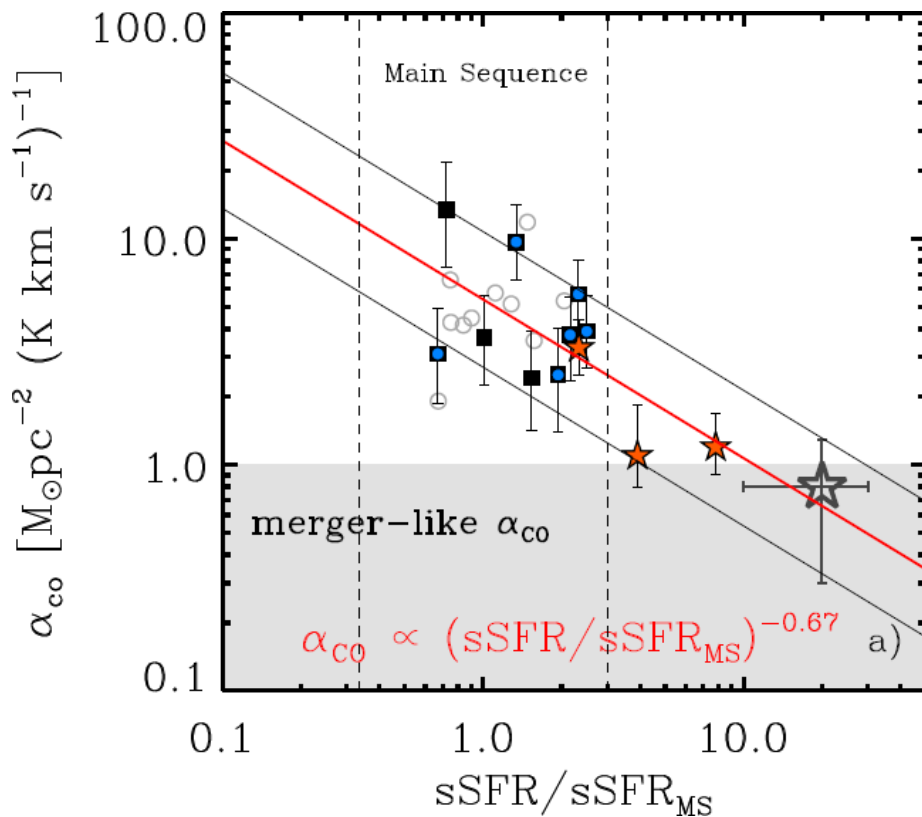
Herschel's Legacy

- Measure: Z , M_{dust} , L_{CO} .
 - Assume $M_{\text{gas}}/M_{\text{dust}}(Z)$ to get α_{CO} .
 - Assume $\alpha_{\text{CO}}(Z)$ to get $M_{\text{gas}}/M_{\text{dust}}$.



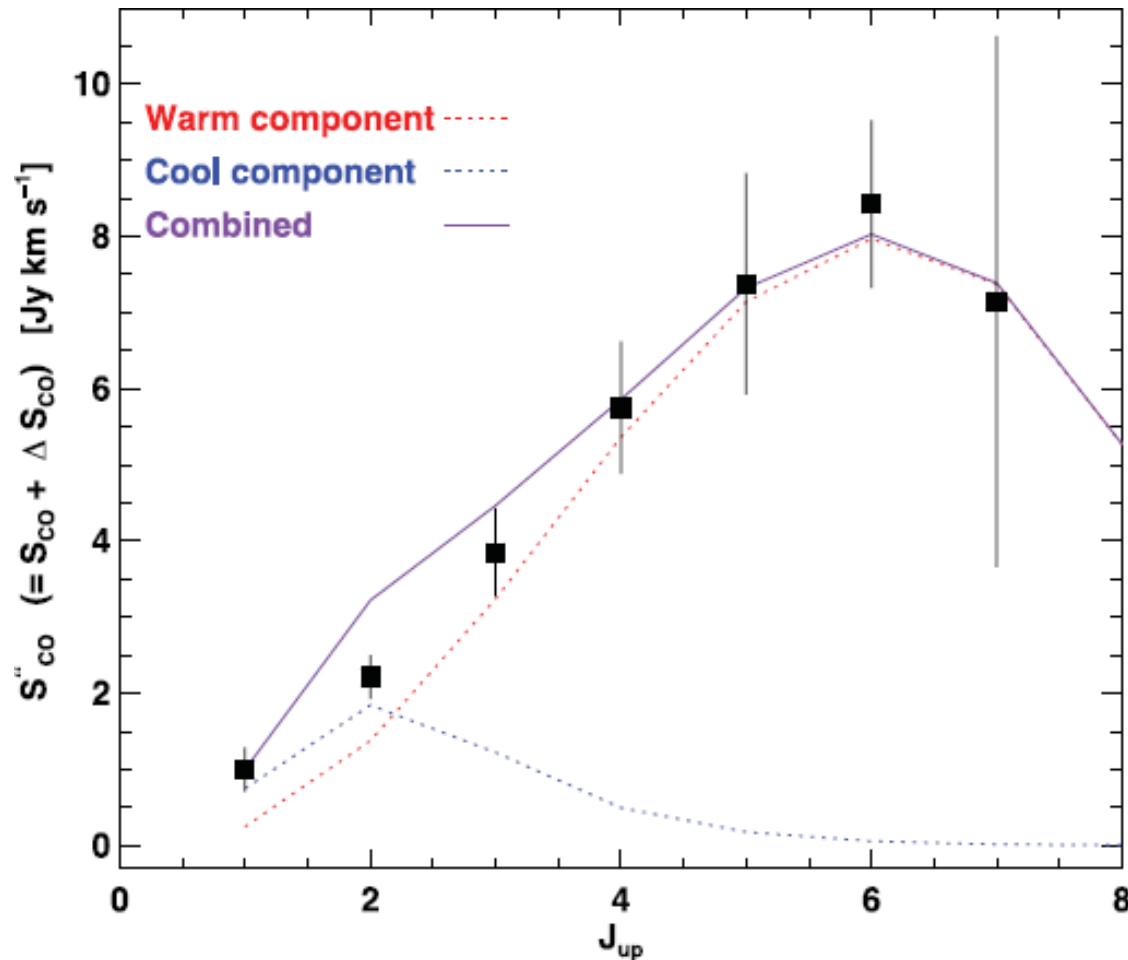
Herschel's Legacy

- What happens with $X_{\text{CO}}/\alpha_{\text{CO}}$ at high star formation rates is still an open question.
- T_B may/should be higher due to gas-to-dust coupling.



Pandora³ Box

- Sub-millimeter Galaxies (SMG) at $z=2.2$: most of CO emission is **not** in CO(1-0)!



The End



Title

- Text