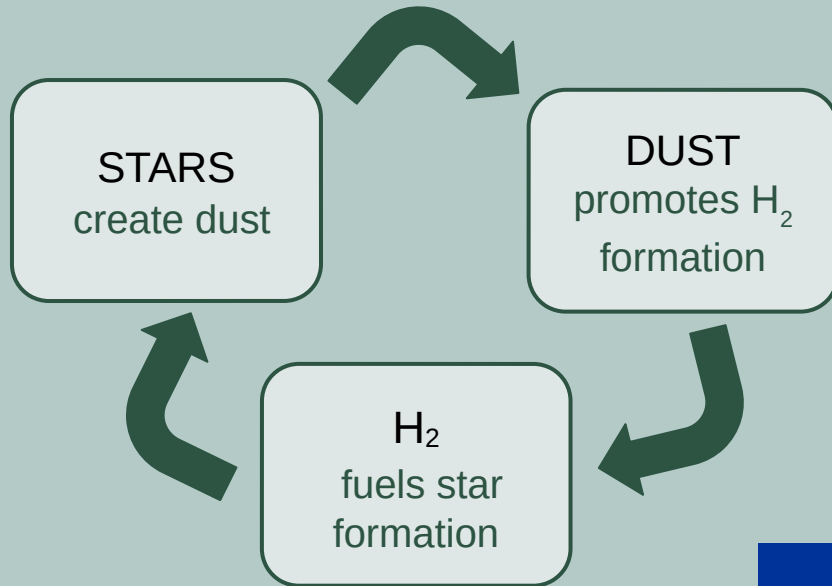


Intertwined Formation of H_2 , Stars, and Dust in Cosmological Simulations



Cynthia Ragone-Figueroa
Also starring...
GL Granato, M. Parente,
G. Murante, M. Valentini
S. Borgani, U. Maio

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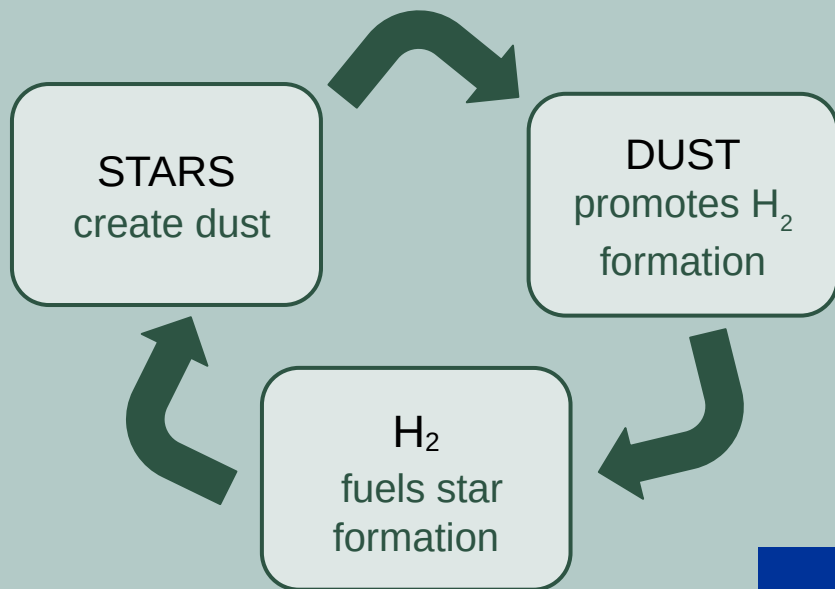
GL Granato, M. Parente,

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Disclaimer:

No OpenGADGET3 here,
P-GADGET+MUPPI instead



StarDust formed in Stellar Outflows

The ejected material from stars (AGBs & SNe), enriched with heavy elements like C, Si, O, and Fe, cools and condenses into solid particles: **StarDust**

Dust is a very active element in the ISM

- ✓ Modifies the radiation field
- ✓ Enhances radiative pressure
- ✓ Contributes to hot gas ($>10^6\text{K}$) cooling

✓ ...
Catalyzes H_2 formation

Once in the ISM...

Mass Change

Accretion

in addition to *stardust*, grains can grow by *accretion* (atoms and ions deposited on cold grain surfaces)

M
A
S
S

Dust Destruction SN shocks & Thermal Sputtering

(collision w energetic ions, hot phase 10^6K)

M
A
S
S

Size Change

Coagulation

In dense clouds Small grains stick together during low velocity collisions ($\sim 0.1\text{ km/s}$), to create Large grains

S
I
Z
E

Shattering

Large grains fragment in high velocity collisions ($>10\text{ km/s}$)

S
I
Z
E

STARS
create dust

DUST

H_2
fuels star
formation

Astration

Dust Promotes H₂ Formation

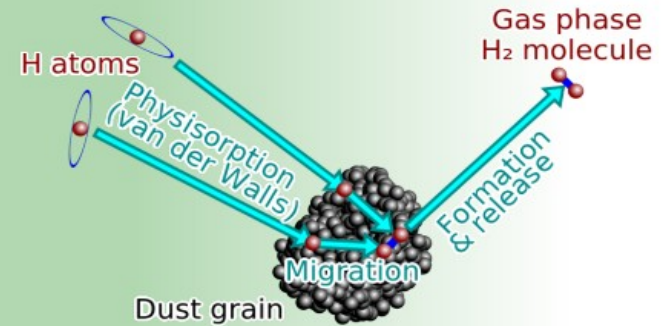
STARS
create dust

DUST
promotes H₂
formation

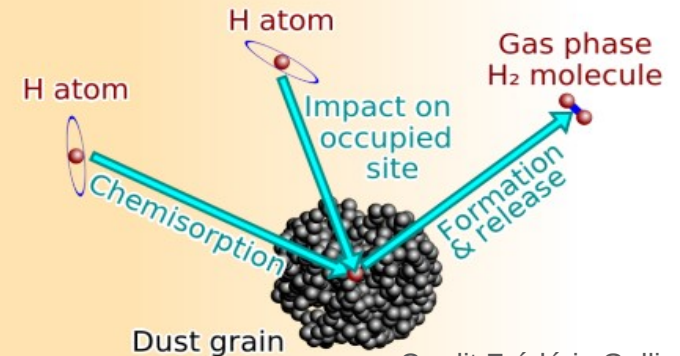
H₂

- Direct H₂ formation in gas very inefficient due to H₂ molecule difficulty to radiate away the excess energy. Relevant only in primordial conditions.
- When H atoms meet and form H₂ on a grain, the grain structure absorbs the excess energy and the molecule stabilizes.
- It takes place primarily on small grains.
- The most abundant molecule in the Universe is H₂.
Molecular Clouds are made of H₂+He+a few % metals (gas and dust)

(a) LANGMUIR-HINSHELWOOD



(b) ELEY-RIDEAL



Credit Frédéric Galliano

Molecular Clouds as Bricks for Star Formation

Timescales:

5-20Myr before the onset of intense high-mass SF

Fast <5Myr clearing of gas before the first SNe

Lifetime: 20-40Myr for M33, Miura+ (2012)

Lifetime: (27 +/- 12) Myr for MW, Murray (2011)

Schinnerer & Leroy 2024

SCHEMATIC VIEW OF MOLECULAR CLOUD EVOLUTION



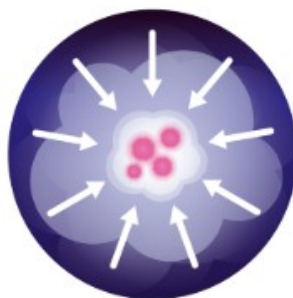
molecular cloud

cloud begins as an over-density of cold gas (predominantly H₂)



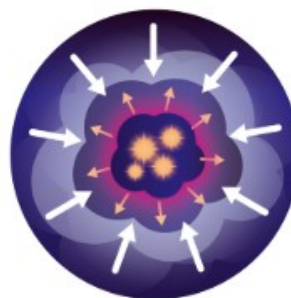
dense gas formation

A subset of the gas achieves high column and volume densities



onset of star formation

Stars form from this dense material.



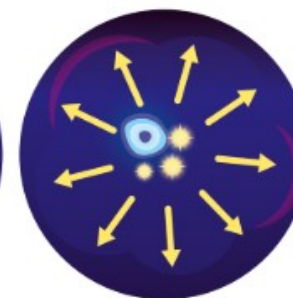
pre-supernovae stellar feedback

pre-SN: gas clearing by winds, radiation, and thermal gas pressure



cloud disruption

Newly formed massive stars rapidly impact their surrounding birth material via radiation and winds, reshaping or even disrupting the cloud



cloud dispersal & supernova explosions

STARS

DUST promotes H₂ formation

H₂ fuels star formation

Molecular Clouds as Bricks for Star Formation

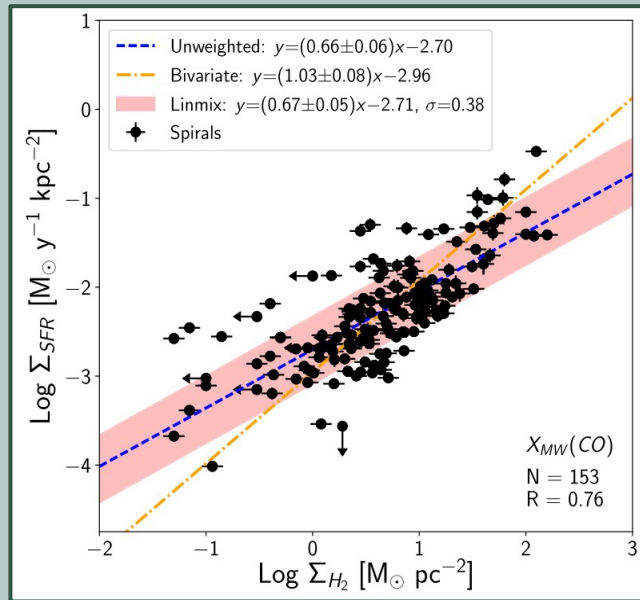
STARS

DUST
promotes H₂
formation

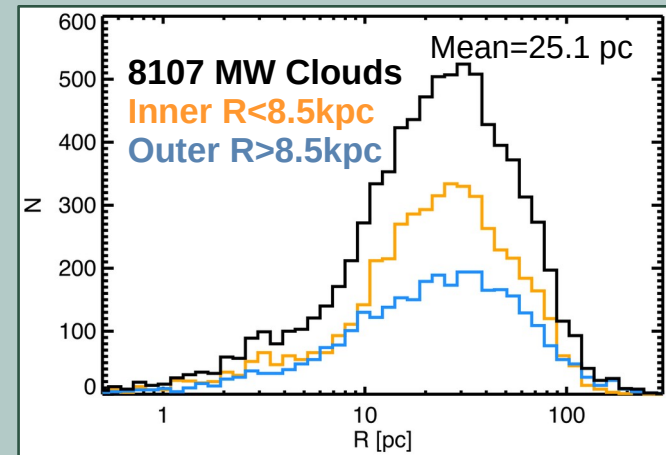
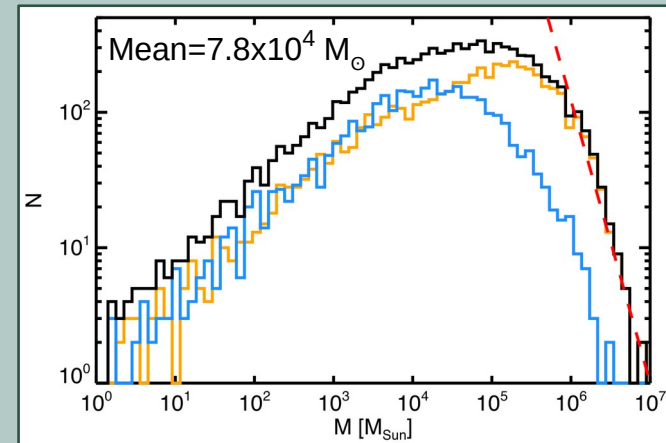
H₂
fuels star
formation

H₂ is the Main constituent of
Molecular Clouds

- ✓ MCs are the densest and coldest component of the ISM
- ✓ Very complex entities
 - Gravitation
 - Magnetic fields
 - Heating & Cooling
 - Turbulence & Shocks



De los Reyes & Kennicutt (2019)



Miville-Deschenes, Murray & Lee, 2017

Molecular Clouds as Bricks for Star Formation

STARS

DUST
promotes H₂
formation

H₂
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H₂ is the Main constituent of
Molecular Clouds

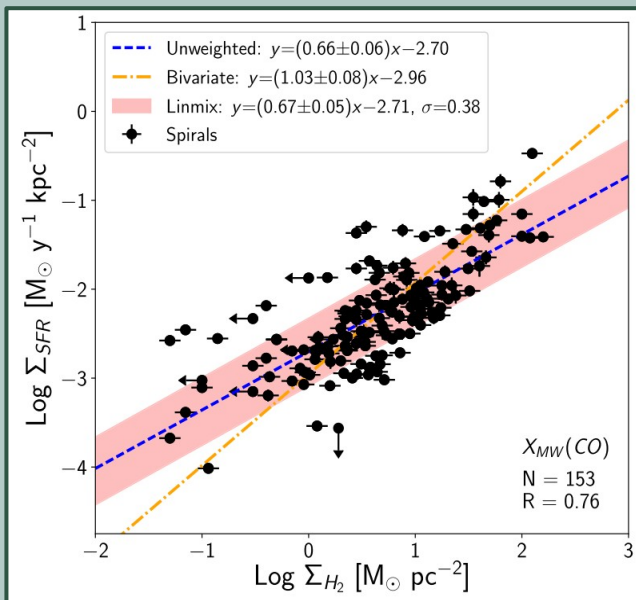
- ✓ MCs are the densest and coldest component of the ISM
- ✓ Very complex entities
 - Gravitation
 - Magnetic fields
 - Heating & Cooling
 - Turbulence & Shocks

Typical Masses: $10^4 - 10^5 M_{\odot}$
Typical Sizes: 20 - 30 pc

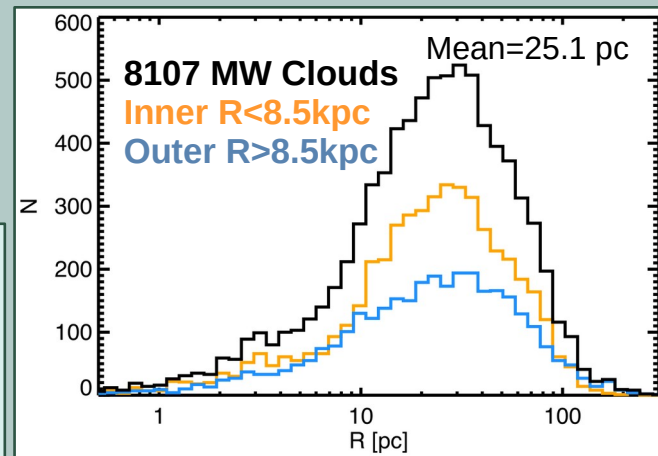
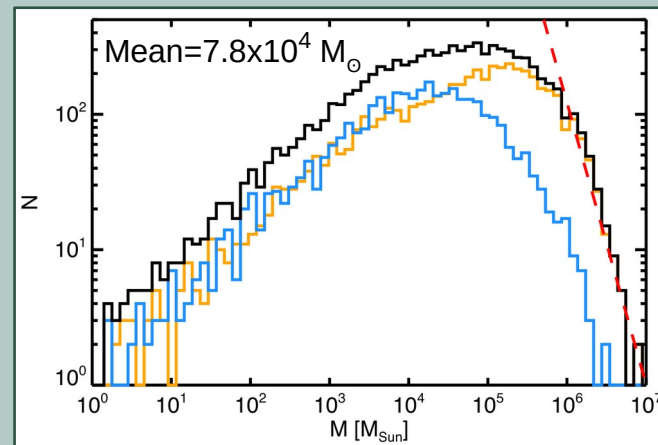
**Not Resolved in
Cosmological
Simulations**

Cosmological
simulations cover a
volume of at least a
few (tens of) Mpc

SF modeling from first principle is
impossible in this context due to
complex physical mechanisms across
vast scale range (> 10 orders of
magnitude in size).



De los Reyes & Kennicutt (2019) INTEGRATED



Miville-Deschenes, Murray & Lee, 2017

Mass and energy transfers between phases in MP particles regulated by simple differential equations describing cooling, star formation and feedback"s". *SAM-like*

Murante+10,15

MUPPI (MULTI Phase Particle Integrator)

A subgrid model for Star Formation and Feedback"s"

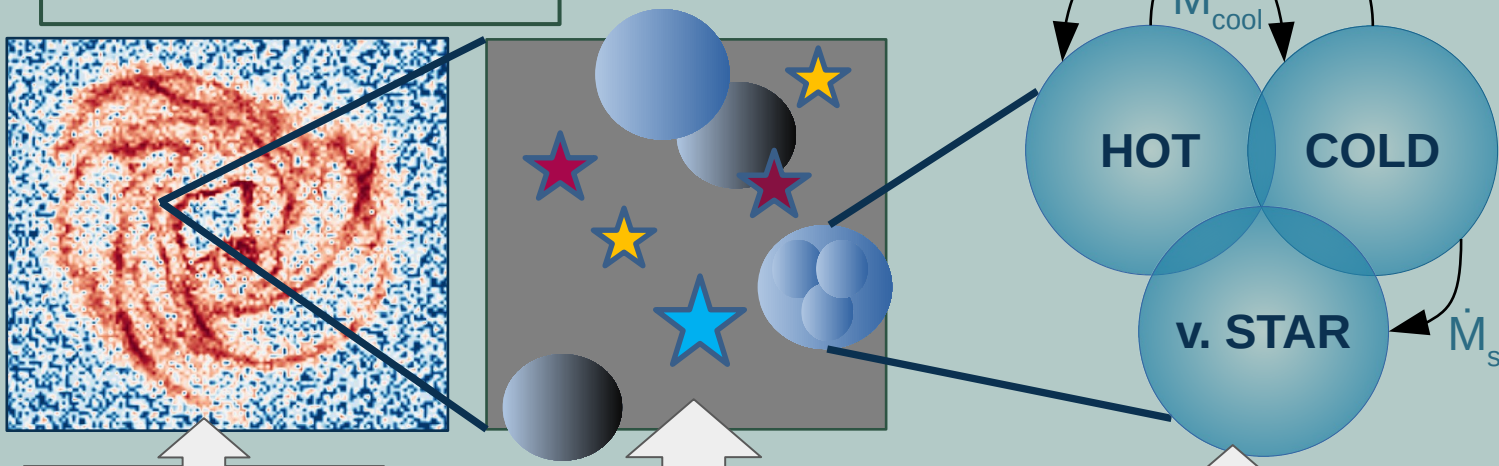
MUPPI mass flows differential equations:

$$\dot{M}_* = \dot{M}_{sf}$$

$$\dot{M}_c = \dot{M}_{cool} - \dot{M}_{sf} - \dot{M}_{ev} - \dot{M}_{AGN}$$

$$\dot{M}_h = -\dot{M}_{cool} + \dot{M}_{ev} + \dot{M}_{AGN}$$

AGN, Valentini+20



A simulated galaxy

a bunch of particles
DM, stars, gas

A Multi-Phase gas particle
 $n > 0.01\text{cm}^{-3}$
 $T < 5 \times 10^4\text{K}$

$$\text{SFR} = \epsilon \times M_{\text{MOL}} / t_{\text{dyn,c}}$$

ORIGINAL MUPPI

Mass and energy transfers between phases in MP particles regulated by simple differential equations describing cooling, star formation and feedback"s". **SAM-like**

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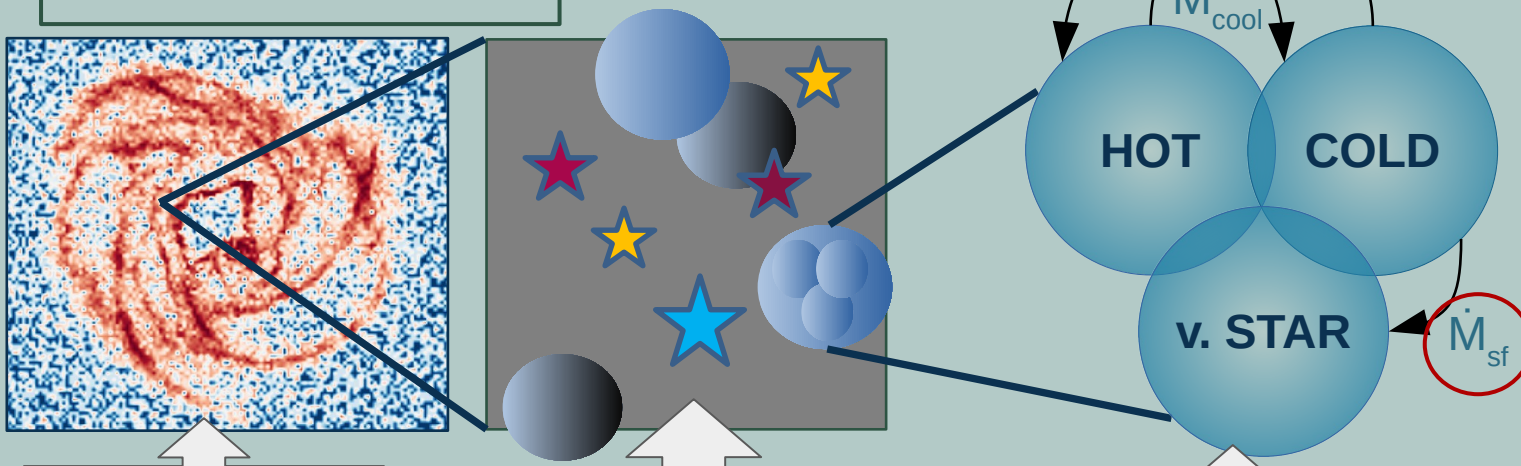
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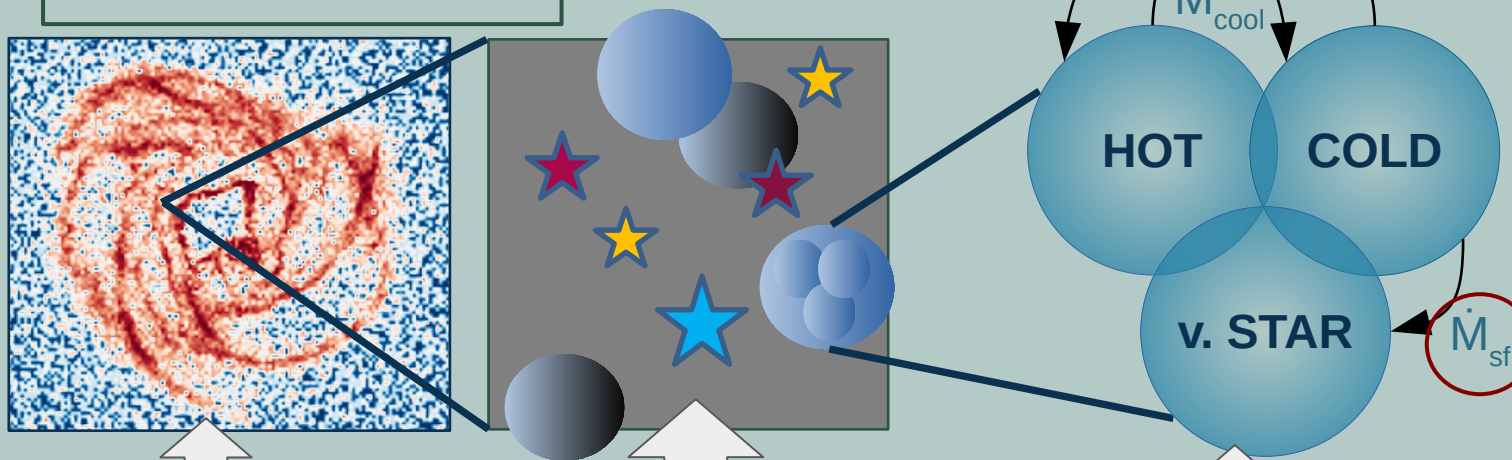
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?

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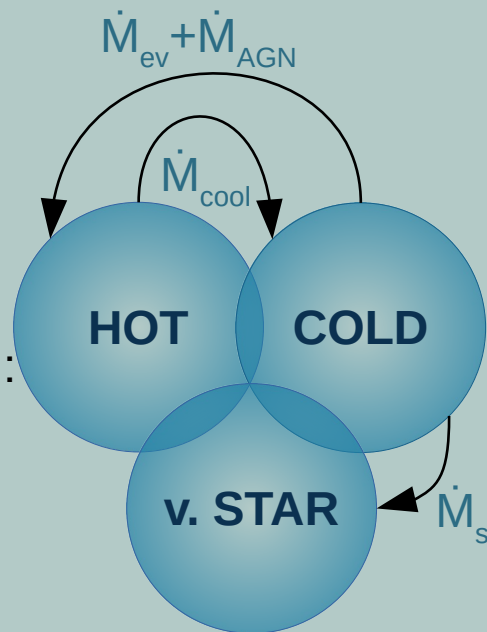
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AGN, Valentini+20



?

$f_{mol} := M_{MOL} / M_{COLD}$ estimated by a prescription:

$$f_{mol} = \frac{1}{1 + P_0/P}$$

$$SFR = \epsilon \times M_{MOL} / t_{dyn,c}$$

$f_{mol} = f_{mol}(P)$ "inspired" by **Blitz, Rosolowsky+ works** (calibrated with **LOCAL** observations)

Alternatively, $f_{mol} = f_{mol}(Z, \Sigma)$ Krumholz+ theoretical works

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Mass and energy transfers between phases in MP particles regulated by simple differential equations describing cooling, star formation and feedback"s". **SAM-like**

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A subgrid model for Star Formation and Feedback"s

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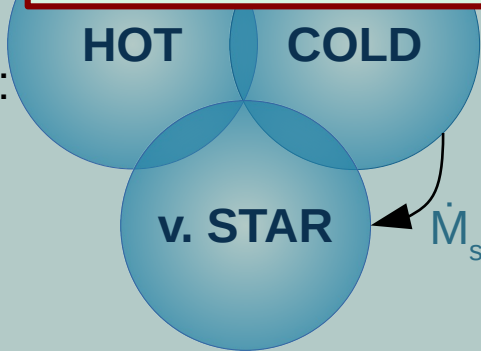
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AGN, Valentini+20

What if we use the H₂ - Star - Dust Cycle instead?

$f_{mol} := M_{MOL} / M_{COLD}$ estimated by a prescription:

$$f_{mol} = \frac{1}{1 + P_0/P}$$



?

$$SFR = \epsilon \times M_{MOL} / t_{dyn,c}$$

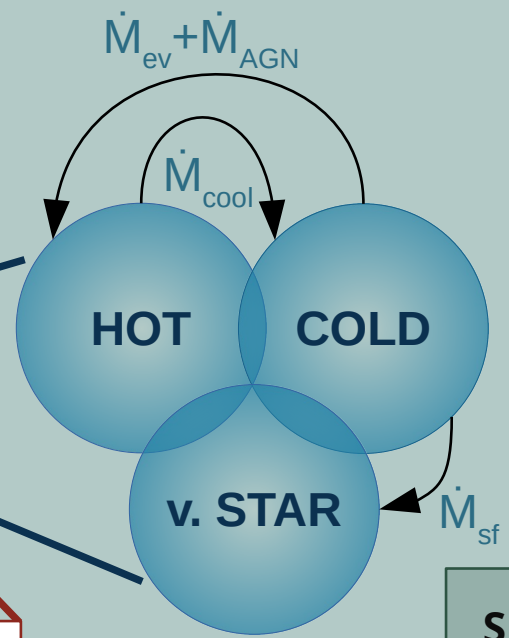
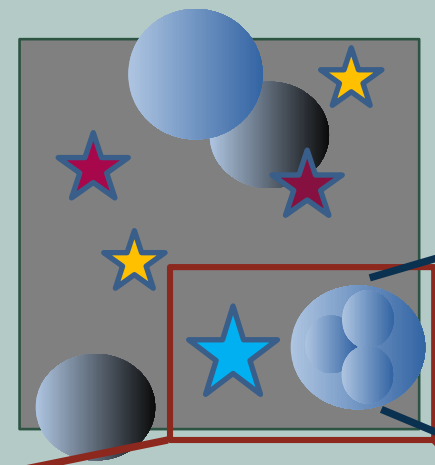
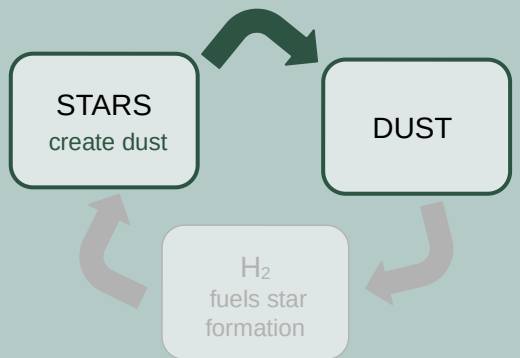
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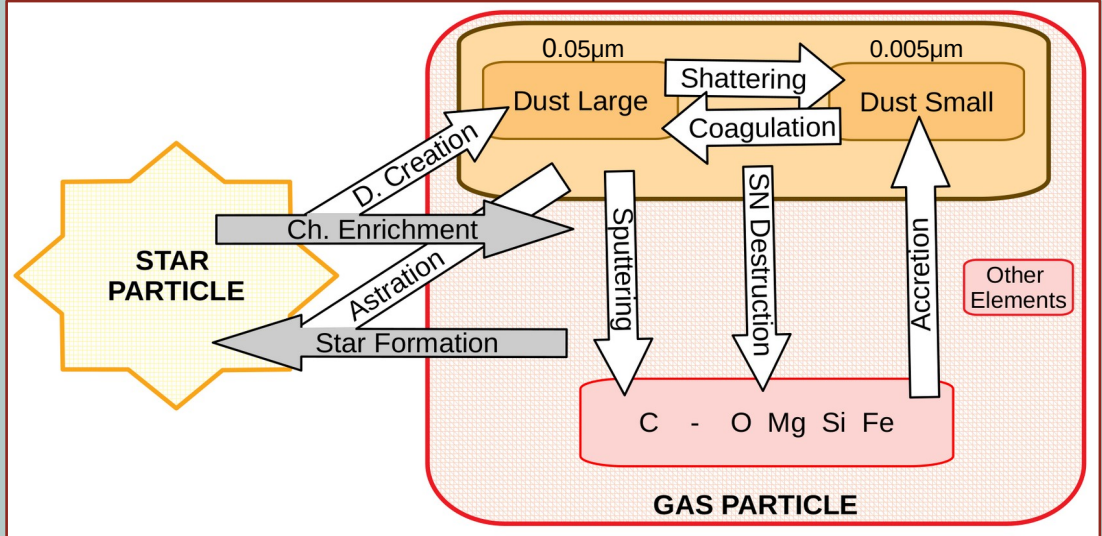
ORIGINAL MUPPI

MUPPI + DUST

Granato+21



Dust Creation & Evolution Model



$$\text{SFR} = \epsilon \times M_{\text{MOL}} / t_{\text{dyn,c}}$$

- ➔ Galaxy Clusters (not MUPPI), Gjergo+18
- ➔ MW-like Galaxies (MUPPI), Granato+21
- ➔ BOX (MUPPI), Parente+22
- ➔ Currently in Open-Gadget (2023, before Sesto)

Dust promoted H₂ CREATION implemented in MUPPI

STARS
create dust

DUST
promotes H₂
formation

H₂
fuels star
formation

fraction of HI atoms that stick,
combine on the surface
of dust grains, and detach
from it as H₂

Dust grains mean geometric
cross-section

Rate of H₂
formation
on dust
grains

Hollenbach & Salpeter (1970-71)

$$R_G = \frac{1}{2} \gamma \langle v_H \rangle n_H n_{gr} \langle \sigma_{gr} \rangle$$

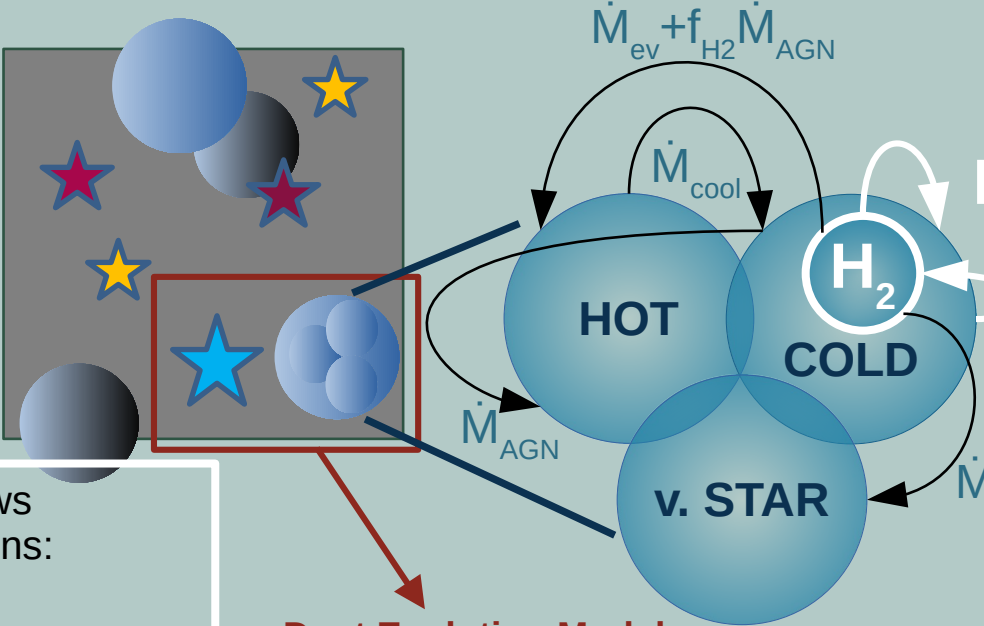
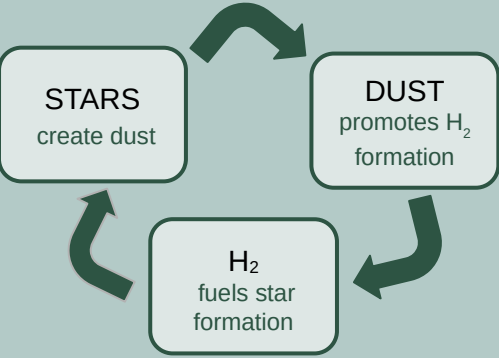
Different Rates for
SMALL and LARGE
grains

Mean velocity of HI atoms

Number density of dust grains

Number density of HI atoms

... and Finally we close the cycle



MUPPI + DUST + H₂
Ragone-Figueroa+24

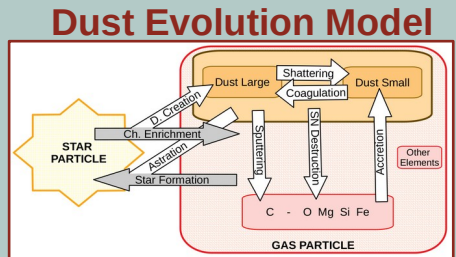
$$R_G = \frac{1}{2} \gamma \langle v_H \rangle n_H n_{gr} \langle \sigma_{gr} \rangle$$

$$SFR = \epsilon \times M_{MOL} / t_{dyn,c}$$



MUPPI mass flows differential equations:

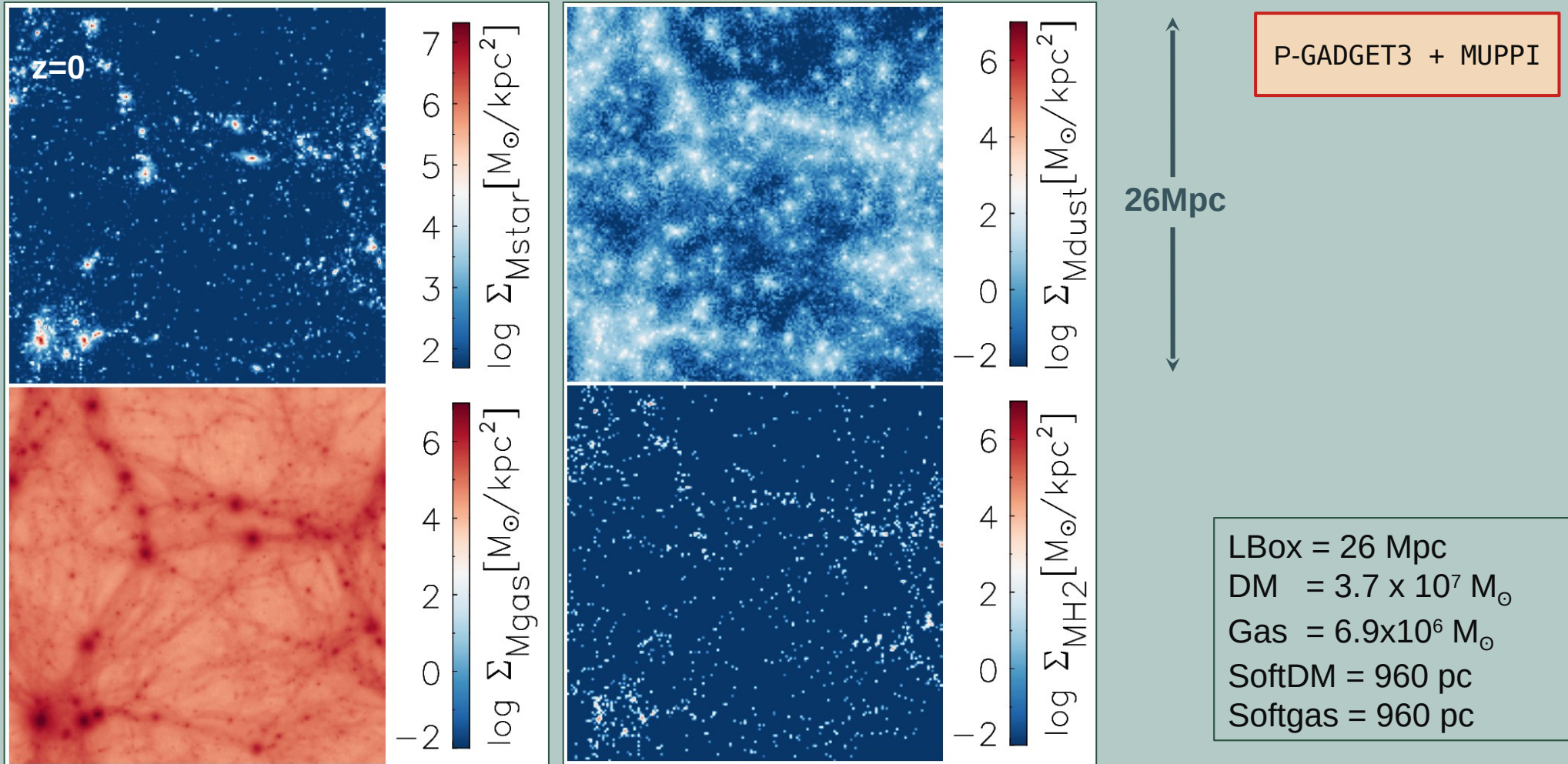
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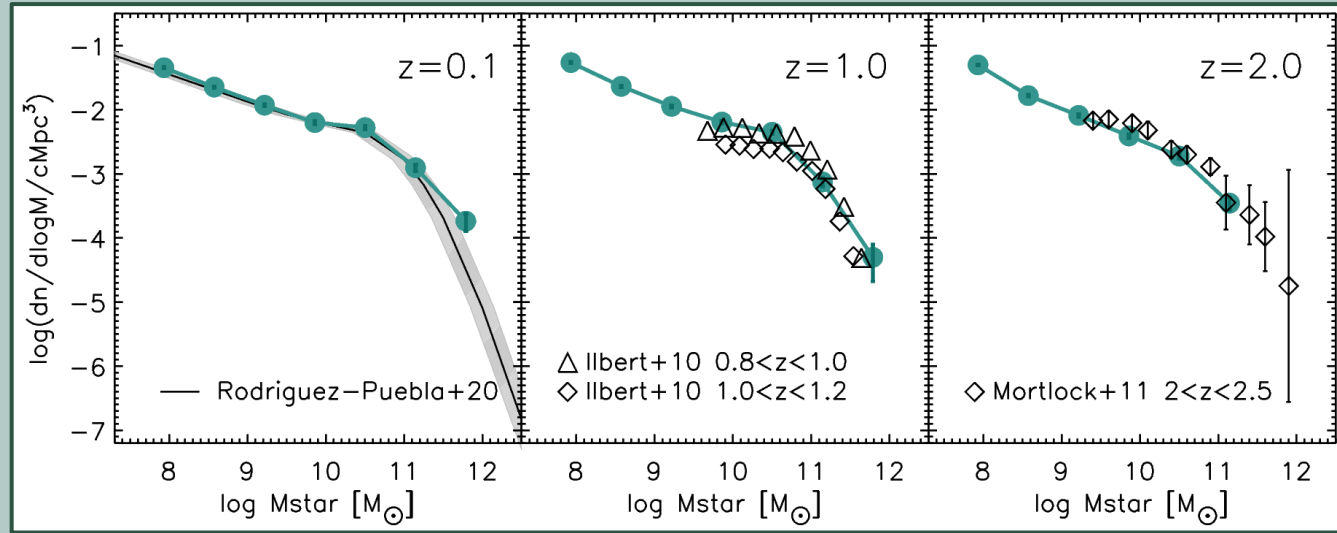
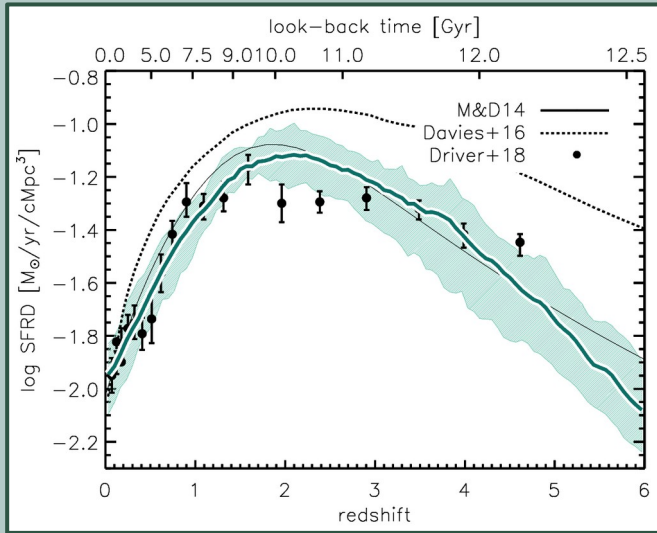
Granato+21 & Parente+22

✓ Now M_{MOL} “self consistently” predicted taking into account $H + H \rightarrow H_2$ on grains

A Visual Inspection: we run 5 boxes like this:

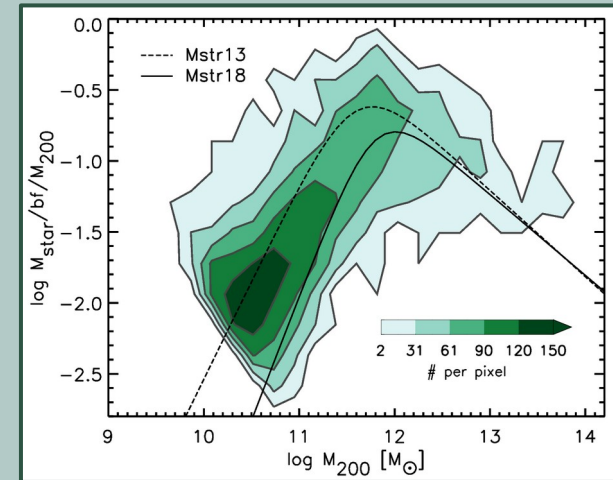


“Calibration Quantities”

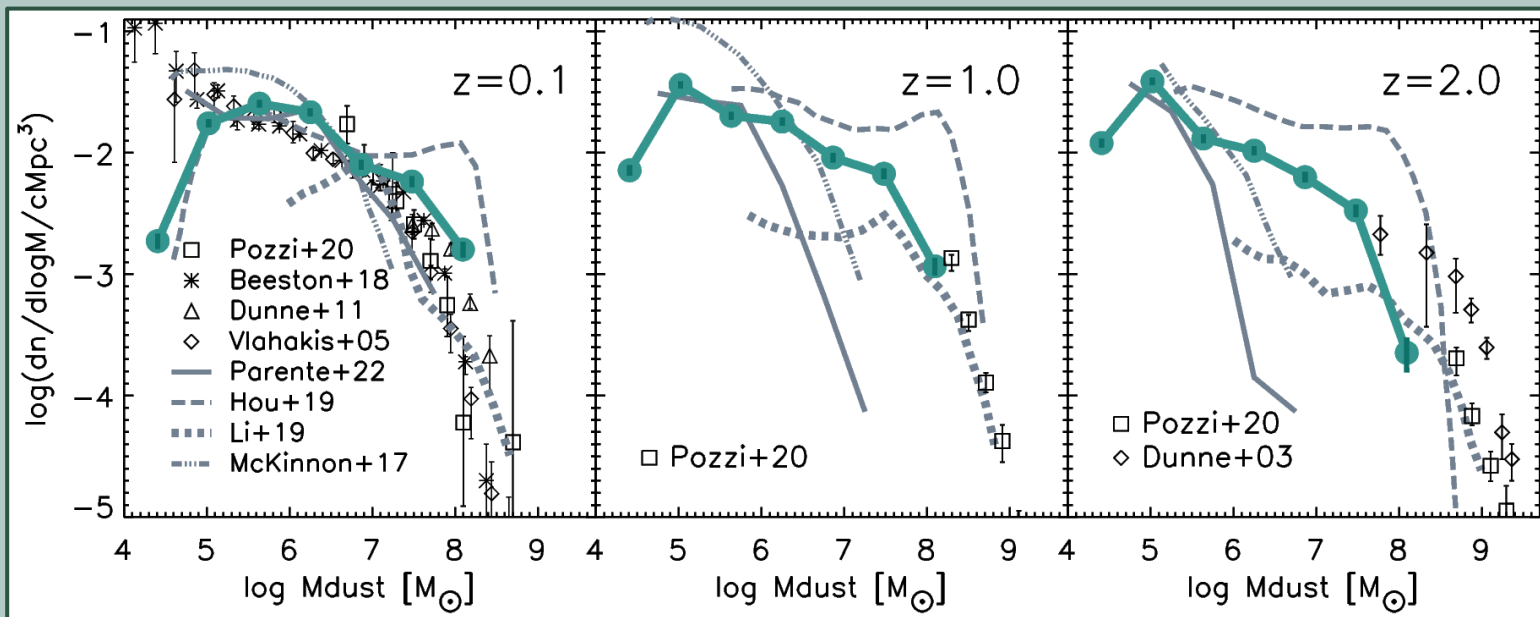


Calibration done using:

- ✓ SFRD
- ✓ Stellar Mass Function @ $z=0$
- ✓ Stellar-Halo Mass @ $z=0$



“Predicted Quantities”: Dust Mass Functions



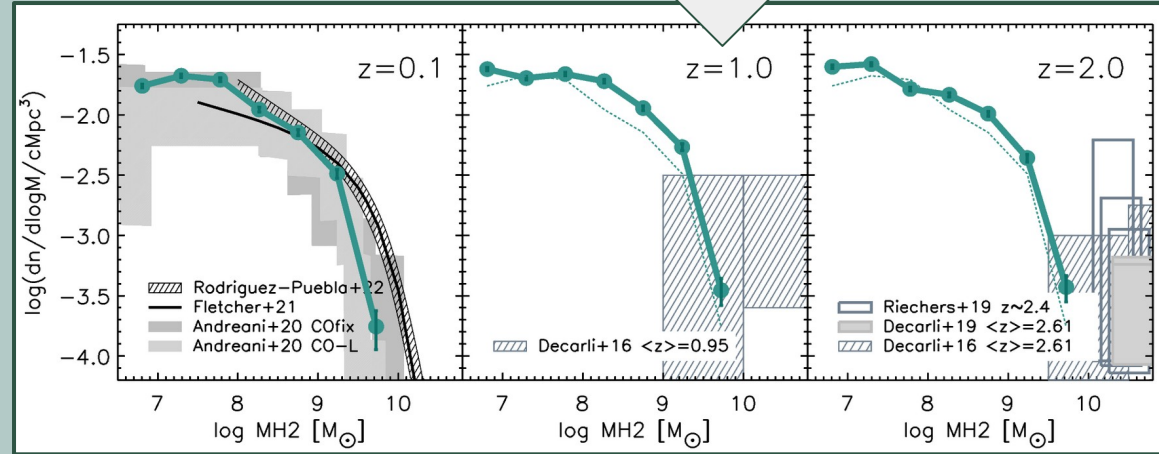
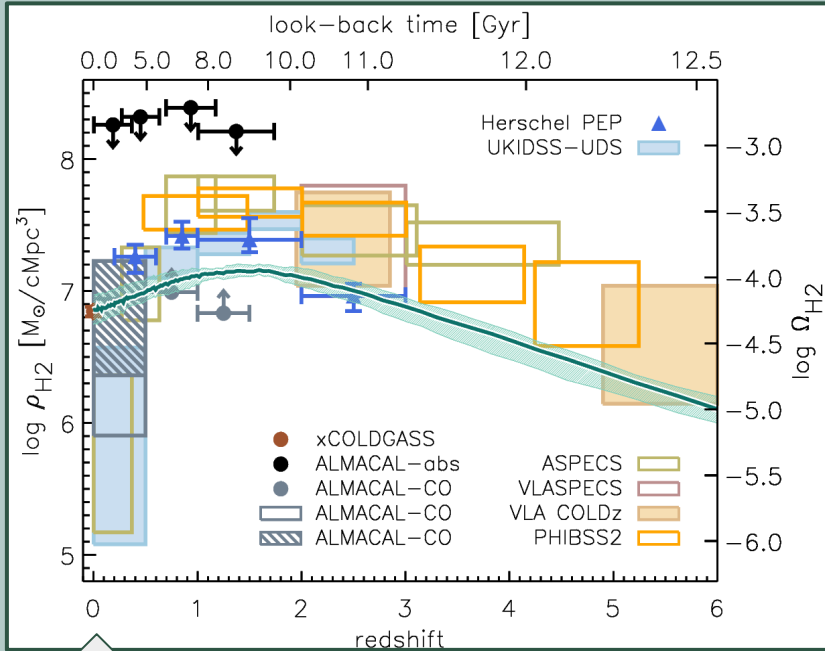
Accurately probing redshifts $z = 1$ and $z = 2$ presents some challenges:

- Observations lack coverage of the small dust masses range that our simulations do sample.
- Conversely, the limited volume of our simulations could lead to an inability to capture the high masses observed in real data, consequently resulting in an under-prediction at the highest dust mass bin.

“Predicted Quantities”: H₂

H₂ is NOT directly observed! (estimated from CO or dust)

H₂ Mass Functions @ z=0, 1, 2



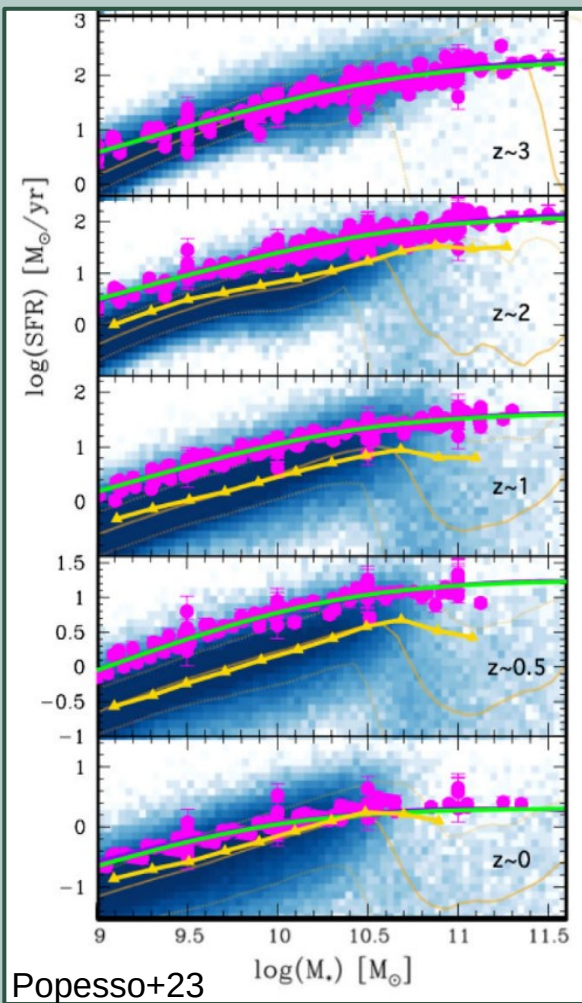
H₂MF shows **little evolution** from z=2 to 0, contrasting with observations (Riechers et al. & Decarli et al., 2019) which report a shift of the characteristic CO luminosity towards lower values of one order of magnitude in the same z range.

CO-, dust-based methods and our model predict a peak at z ~ 1.5 and a decline over the last ~ 9 Gyrs.

Decarli et al. (2019) found that the decline of ρ_{H_2} by a factor of approximately 6 from its peak at z ~ 1.5 to the present would reduce to a factor 3 if they had halved the CO-to-H₂ conversion factor for a galaxies at z>1

H₂
Cosmic
Density

“Predicted Quantities”: the Main Sequence



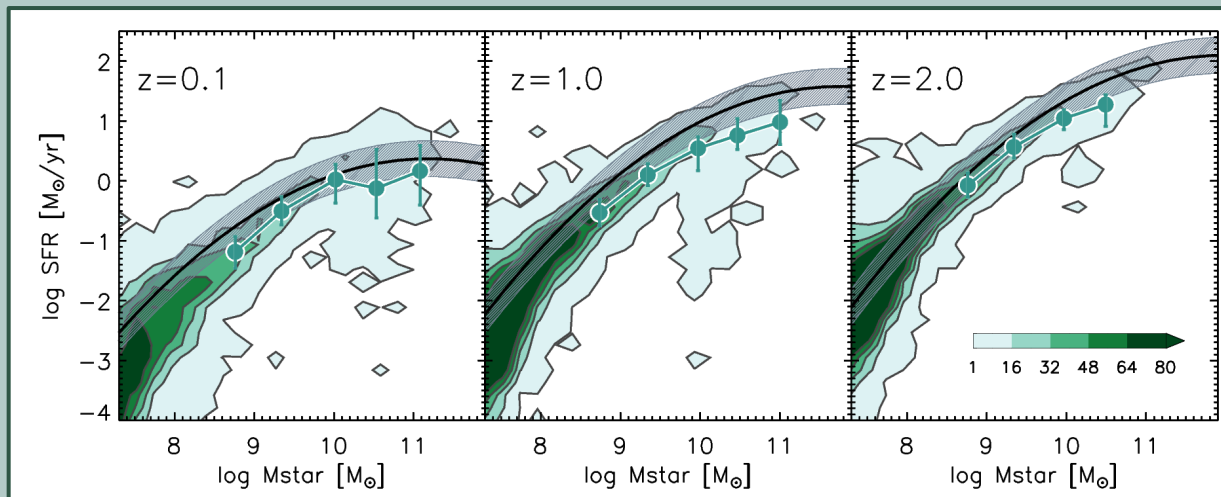
Popesso+23
Observational
Compilation since 2014

Illustris-TNG 300

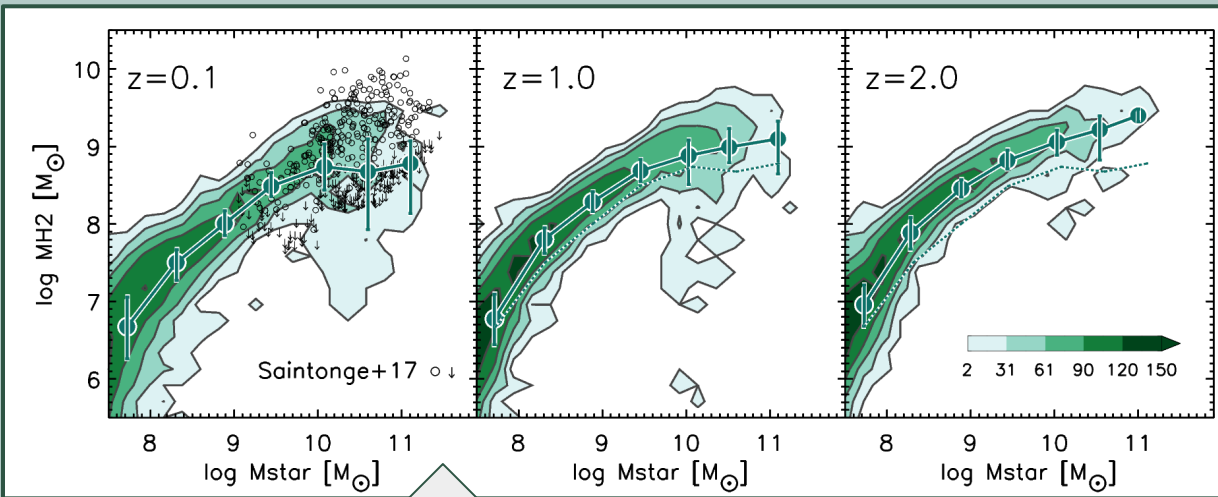
- Median
- ▲ Donnari+19 limited to UVJ selected galaxies

Solid black line: Popesso+23:
The MS bends at high masses.

Green dots: Model Main Sequence
We reproduce the MS bending



“Predicted Quantities”: H₂ scaling relation & the Main Sequence



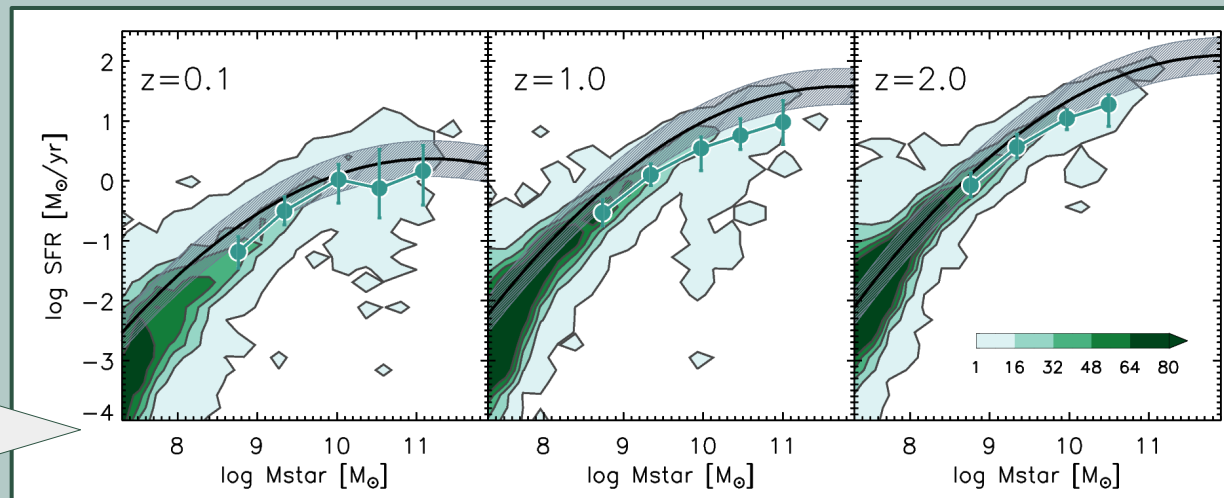
P23: The MS bends at high masses. We reproduce the MS bending.

A similar bending also present in the MH₂-Mstar relation.

Since H₂ is the fuel for SF, the latter implies that the bending of the MS is mainly driven by a relative lack of H₂ in the most massive galaxies.

Mstar vs H₂ mass
(contours and points with dispersion bars are model)

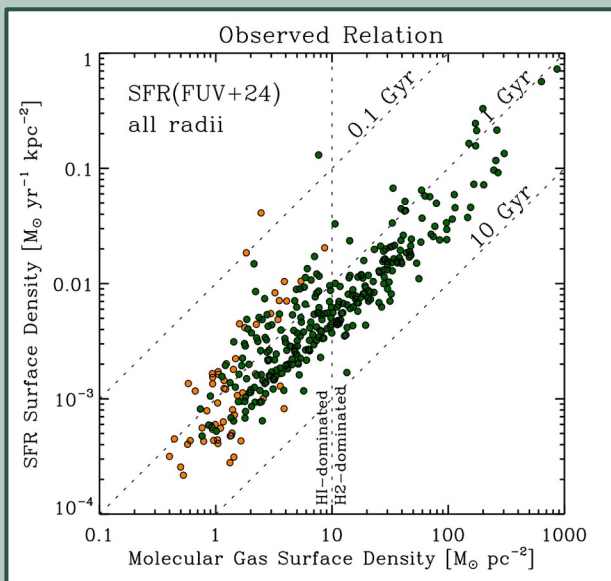
Solid black line: Popesso+23 MS (compilation since 2014)
Green dots: Model MS



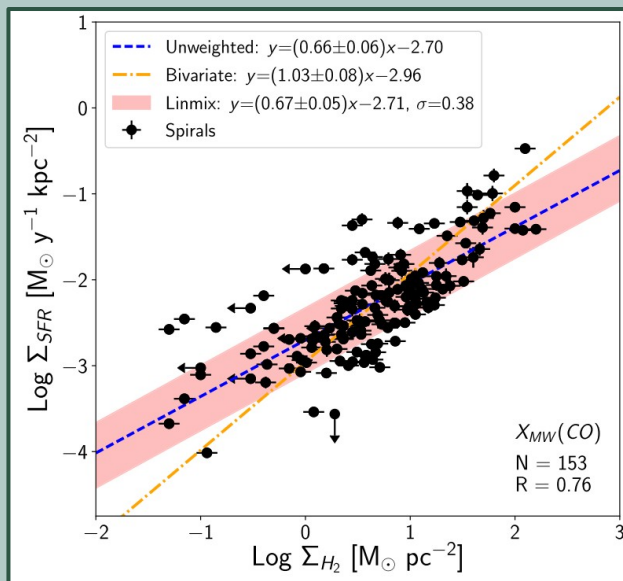
The Molecular Kennicutt-Schmidt Relation

Astronomers have been exploring scaling relationships between gas and star formation since Schmidt's work in 1959.

The question remains:
which gas surface density should be employed?



Schruba et al. (2011) RADIAL



De los Reyes & Kennicutt (2019) INTEGRATED
They compile 114 publications

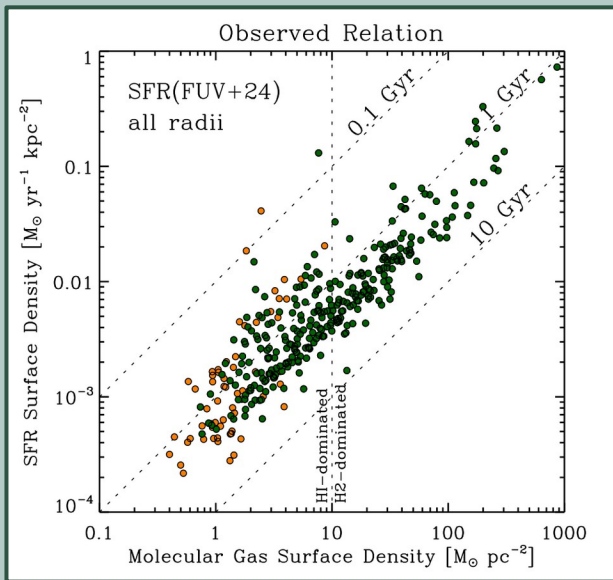
Σ_{H_2}

Wong & Blitz (2002), Kennicutt et al. (2007), Bigiel et al. (2008), Leroy et al. (2008), Wilson et al. (2008), Blanc et al. (2009), Bigiel et al. (2011), de los Reyes & Kennicutt (2019)...

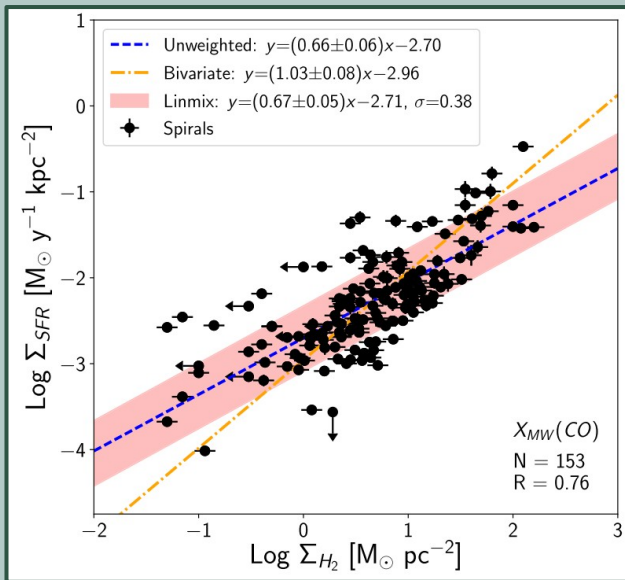
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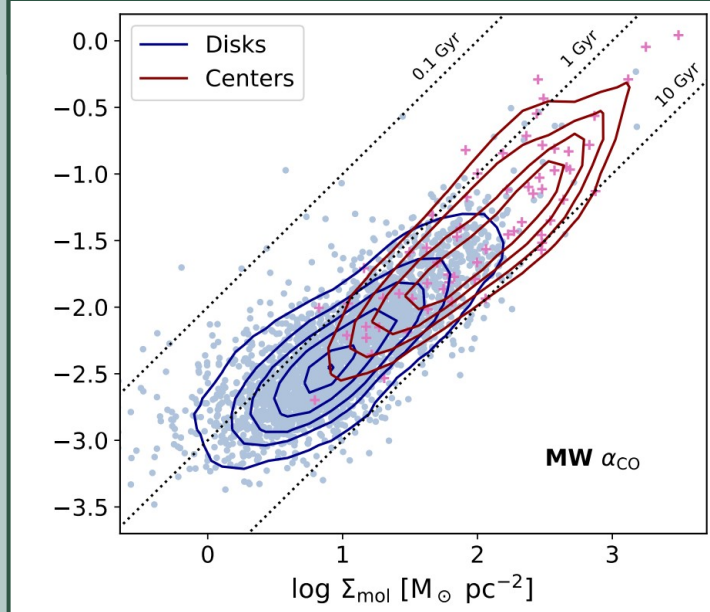
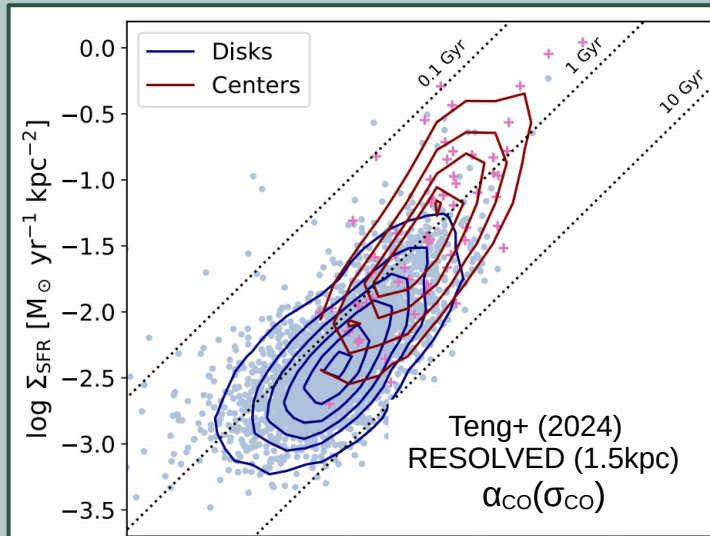
Teng+ (2024): At high Σ_{H_2} , the mKS relation steepens, a phenomenon that goes undetected when a fixed CO-to-H₂ conversion factor is used



Schruba et al. (2011) RADIAL

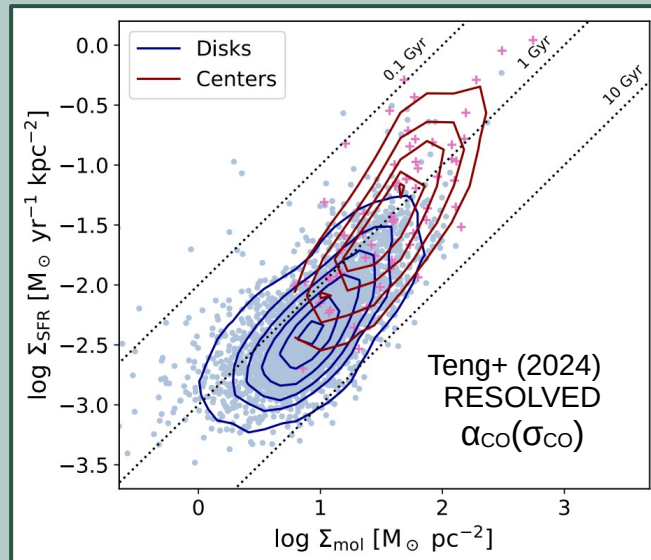
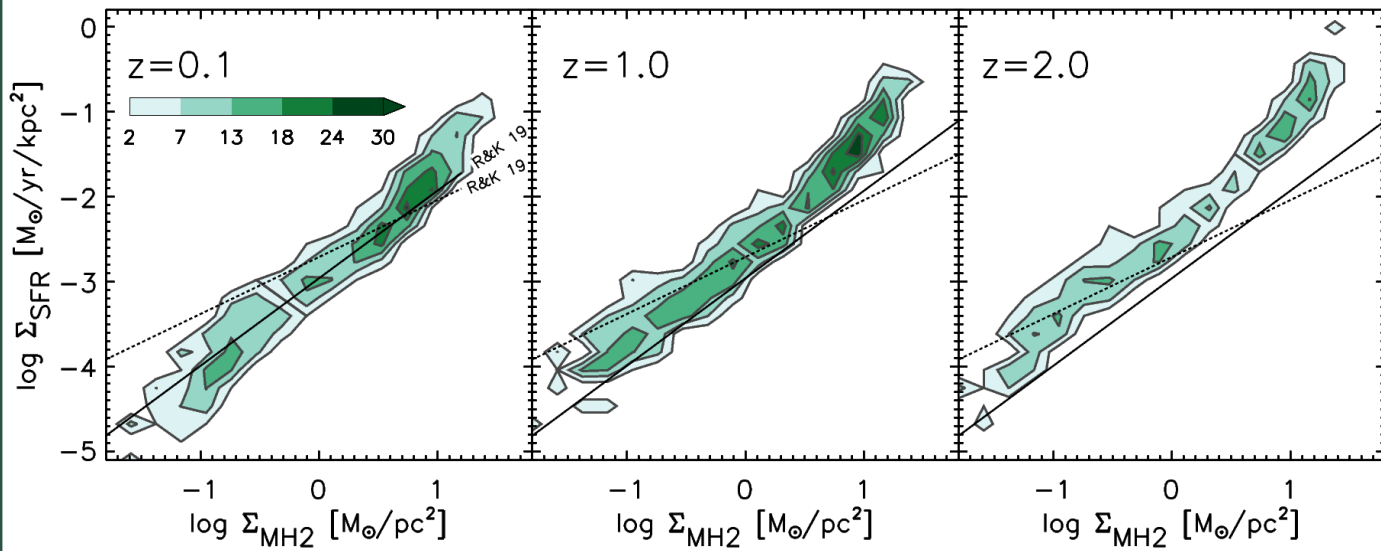


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They compile 114 publications



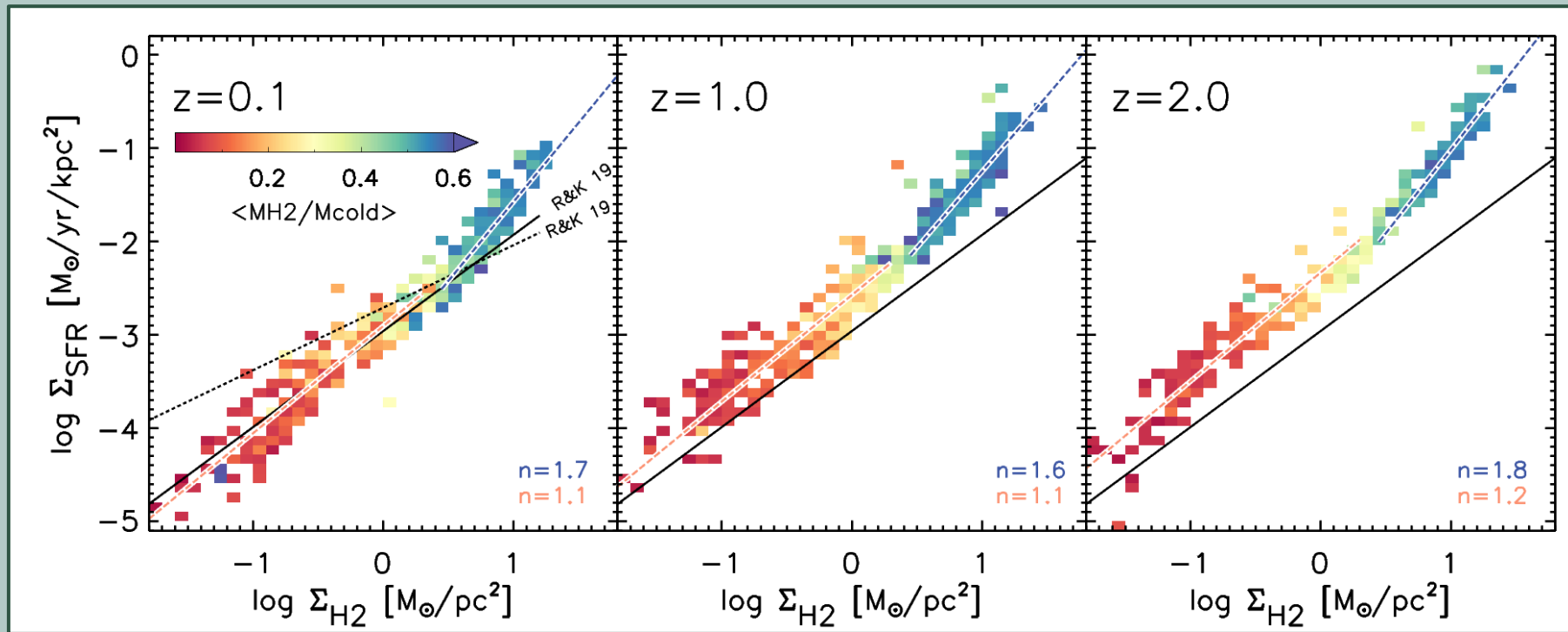
H₂ is NOT directly observed! (estimated from CO or dust)

The Molecular Kennicutt-Schmidt Relation



- ✓ The integrated molecular Kennicutt-Schmidt relation is evident in our model galaxies as early as redshift 2, although with a higher normalization than at redshift 0.
- ✓ The slope remains close to unity across the examined redshifts for surf densities below $\Sigma_{\text{H2}} \sim 5 \text{ M}_{\odot}/\text{pc}^2 \dots$
- ✓ However, at higher surface densities, we observe a steeper slope.

The Molecular Kennicutt-Schmidt Relation



$$\dot{M}_{\text{sf}} = f_* \frac{M_{\text{H}_2}}{(1 - Y)t_{\text{dyn}}}$$

$$t_{\text{dyn}} \propto \rho_c^{-0.5}$$

At high densities

$$\Sigma_{\text{SFR}} \propto \Sigma_{\text{H}_2}^{1.5}$$

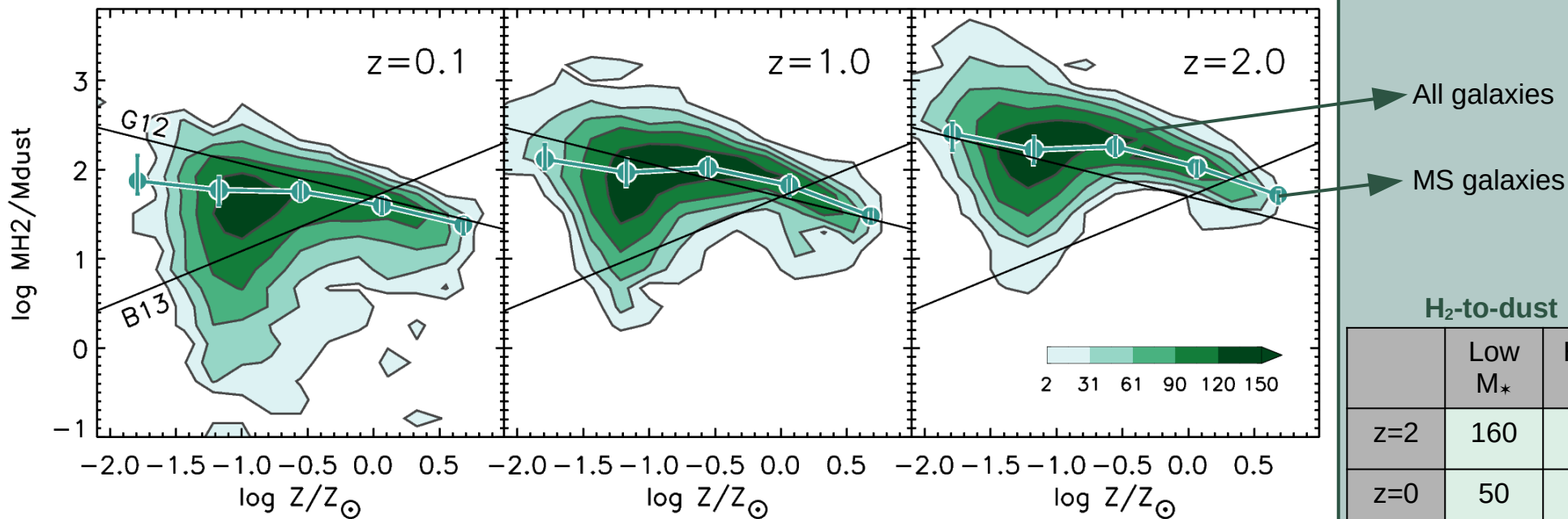
H₂ mass determination from dust: A complex task

The evaluation of molecular mass in galaxies is limited to indirect methods.
 Bertemes+18 derived ($z < 0.2$) a formula to obtain Molecular Mass from Dust Mass:
 G12: Using Genzel+12 CO-to-H₂ conversion factor
 B13: Using Bolatto+13 CO-to-H₂ conversion factor

$$\chi_{G12}(Z) = 10^{-1.27(12 + \log(O/H) - 8.67)},$$

$$\chi_{B13}(Z) = 0.67 \times \exp(0.36 \times 10^{-(12 + \log(O/H) - 8.67)}).$$

G12 sample: MS SF glxs $z > 1$
 + 5 local group glxs,
 $-0.9 < \log(Z/Z_{\odot}) < 0.3$



H₂-to-dust

	Low M_{\star}	High M_{\star}
$z=2$	160	65
$z=0$	50	30

- ✓ Galaxies with higher Z (or M_{\star}) exhibit smaller H₂-to-dust ratios at all redshifts
- ✓ Higher H₂-to-dust dispersion at lower Z (or M_{\star}).
- ✓ Higher normalization associated at higher redshift.

- ✓ G12 determination preferred

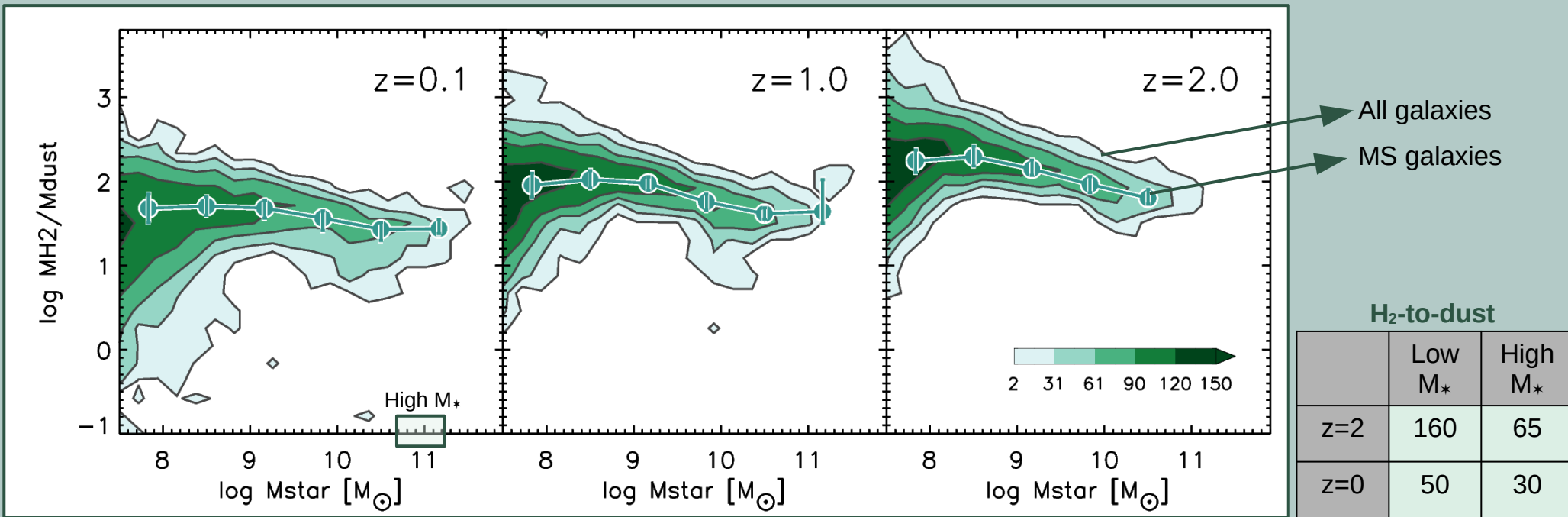
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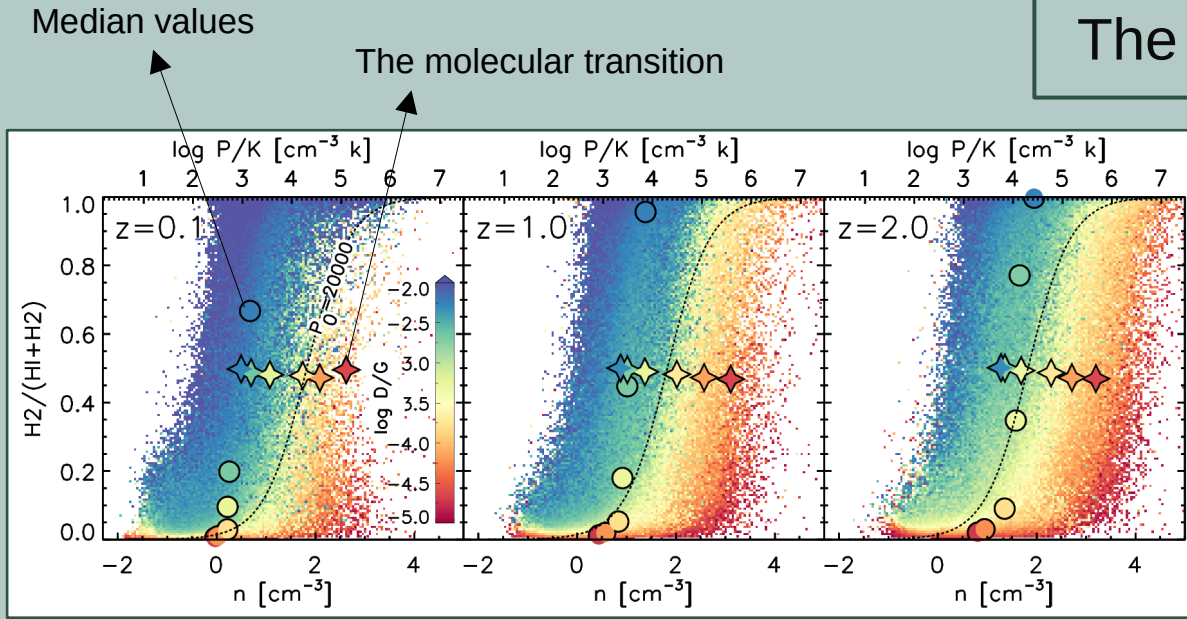
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The atomic to molecular transition

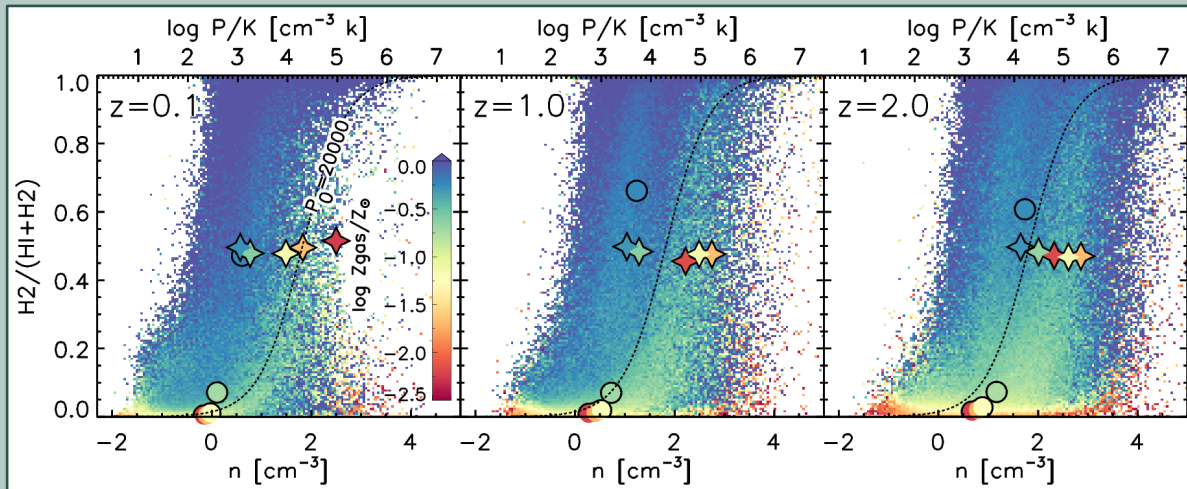


Dust/Gas

At lower D/G the molecular transition occurs at higher densities.

For a given D/G ratio, we recover the B&R “shape”.

Can this prescription be improved?



Metallicity

The atomic to molecular transition is not that clear when using metallicity.

Dust & Metallicity: it is not the same thing

Summary

- In the Universe, Star Formation, Dust pollution and Molecular Gas are intertwined. Now also in these simulations
- **MUPPI Star Formation law is now linked to the dust-promoted H_2 content, which in turn is produced from stellar ejecta and evolves in the ISM**
- We find good agreement with several observational constraints in the range $0 < z < 2$
- The integrated molecular Kennicutt-Schmidt relation emerges as early as redshift $z \sim 2$, although with a higher normalization than at $z=0$.
- Can we improve prescriptions to estimate molecular mass in galaxy formation models, when dust and/or H_2 modeling is not performed

