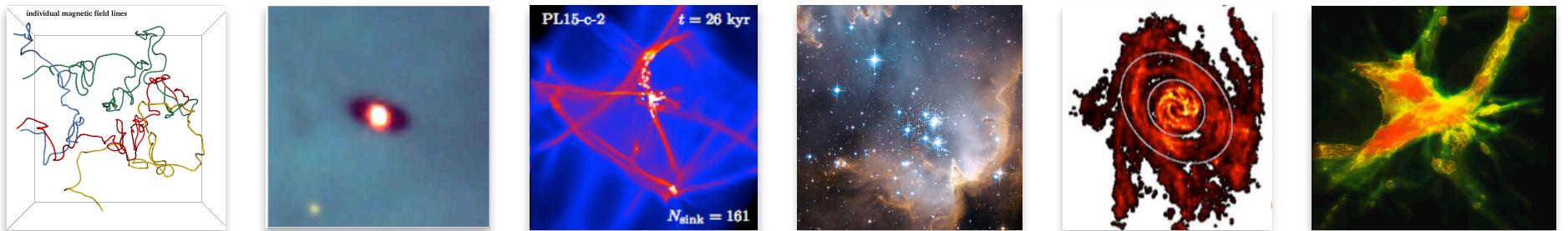


Star Formation

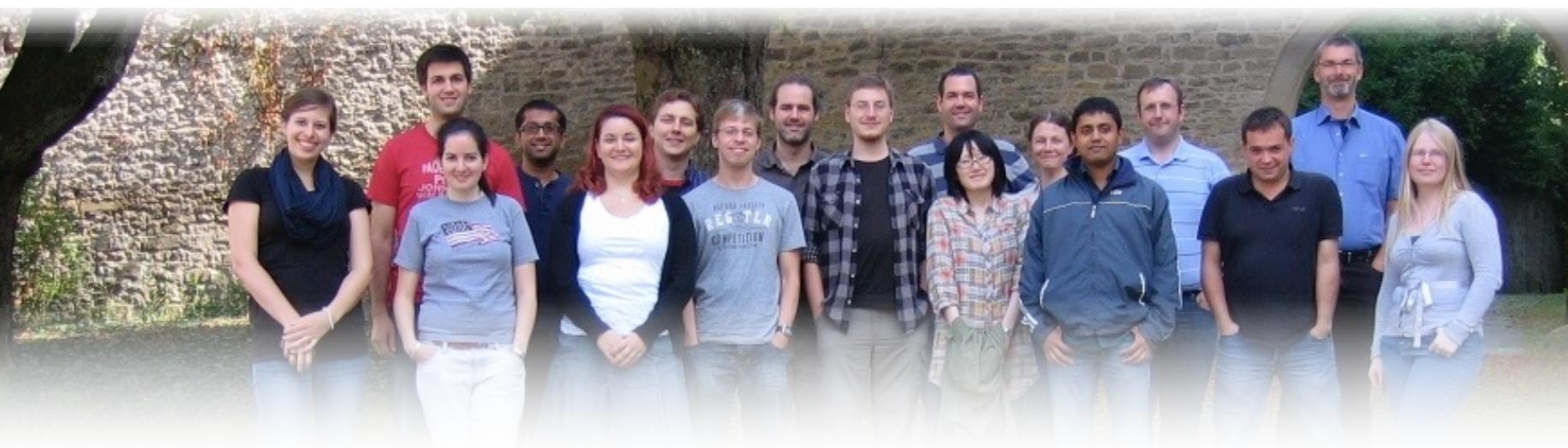


Ralf Klessen

Zentrum für Astronomie der Universität Heidelberg
Institut für Theoretische Astrophysik



thanks to ...



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

Christian Baczyński, 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

... former group members:

Robi Banerjee, Ingo Berentzen, Paul Clark, Christoph Federrath, Philipp Girichidis, Thomas Greif, Milica Micic, Thomas Peters, Dominik Schleicher, Stefan Schmeja, Sharanya Sur, ...

... many collaborators abroad!



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Forschungsgemeinschaft
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WÜRTTEMBERG
STIFTUNG
Wir stiften Zukunft



European
Research
Council

agenda

- star formation theory
 - phenomenology
 - historic remarks
 - our current understanding and its limitations
- applications
 - formation of molecular clouds
 - the stellar mass function at birth (IMF)

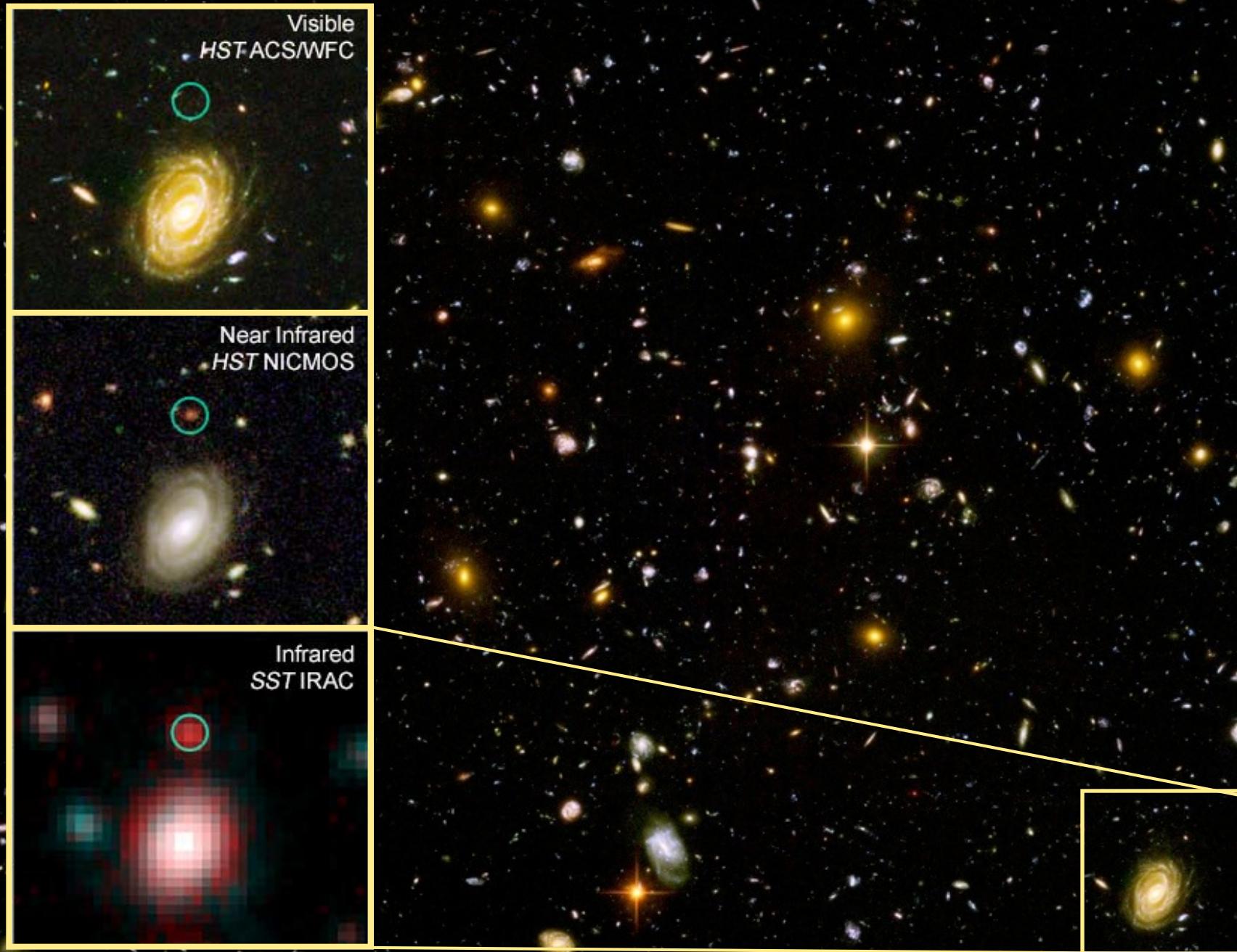


NGC 3324 (Hubble, NASA/ESA)

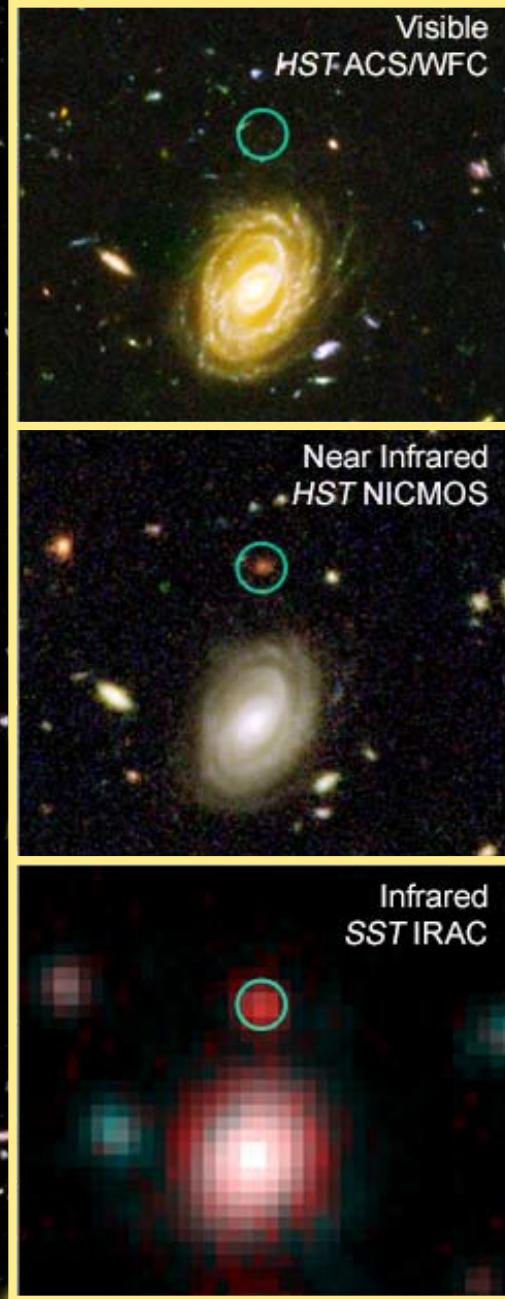
phenomenology



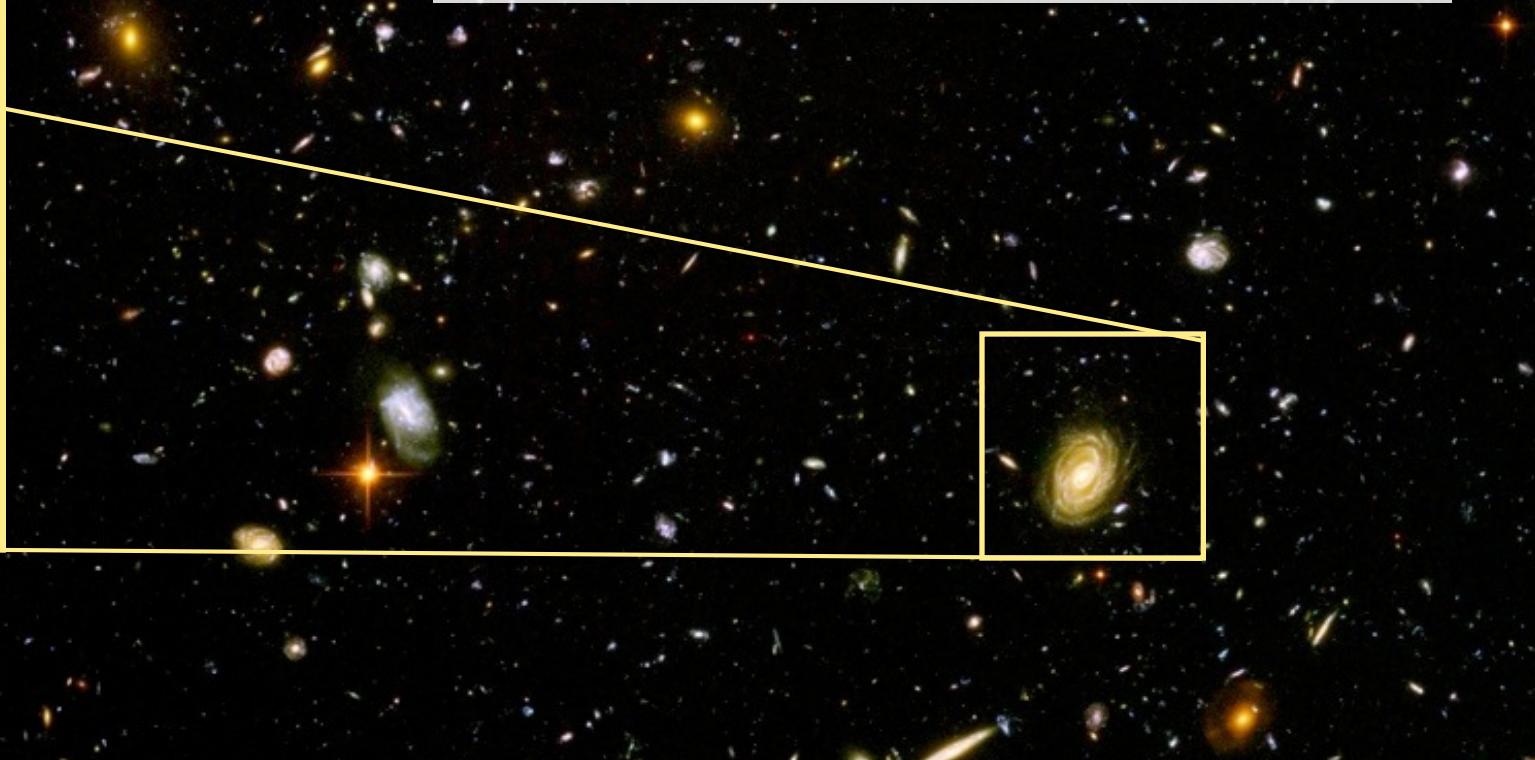
Hubble Ultra-Deep Field



Hubble Ultra-Deep Field

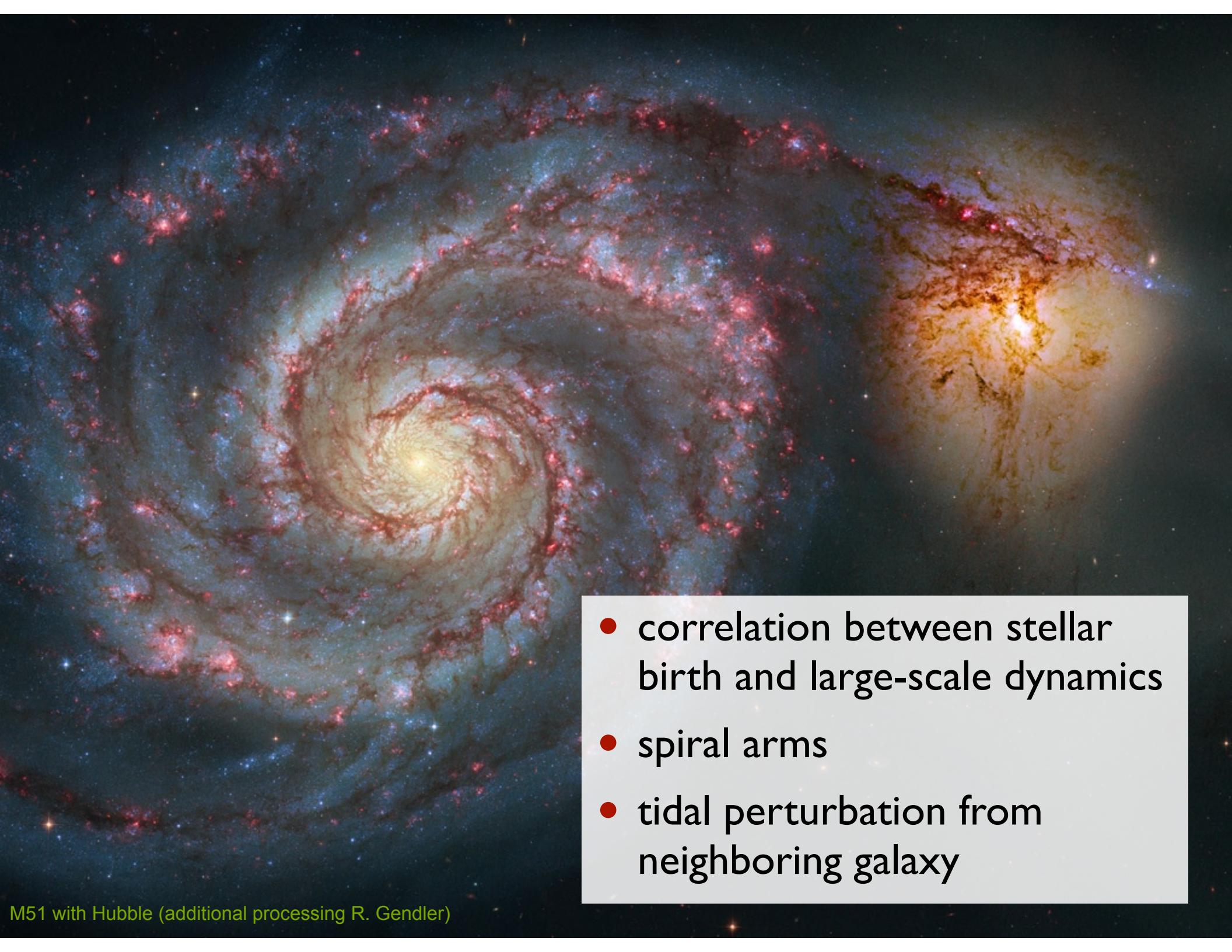


- star formation sets in very early after the big bang
- stars always form in galaxies and protogalaxies
- we cannot see the first generation of stars, but maybe the second one



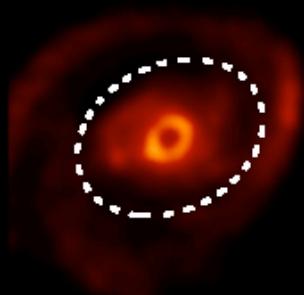


M51 with Hubble (additional processing R. Gendler)

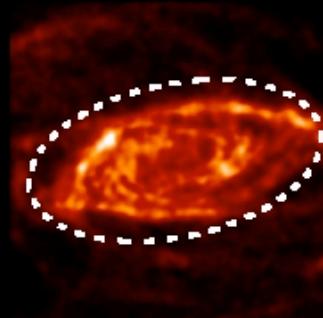


- correlation between stellar birth and large-scale dynamics
- spiral arms
- tidal perturbation from neighboring galaxy

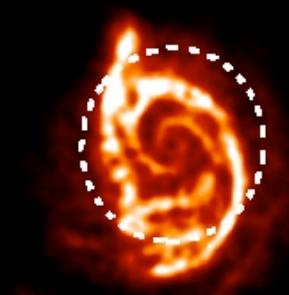
NGC 4736



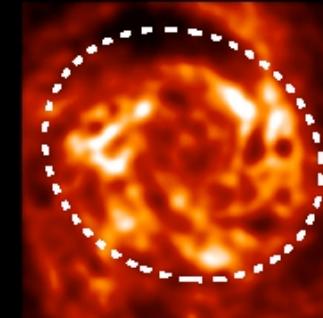
NGC 5055



NGC 5194

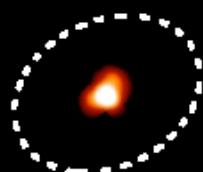


NGC 6946

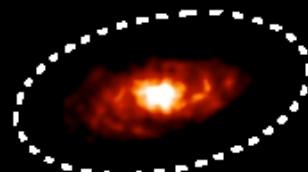


atomic
hydrogen

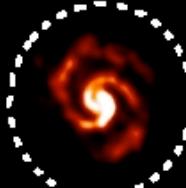
NGC 4736



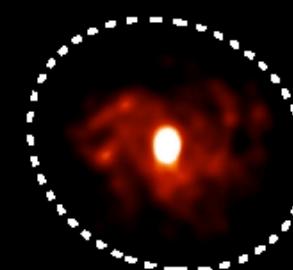
NGC 5055



NGC 5194



NGC 6946

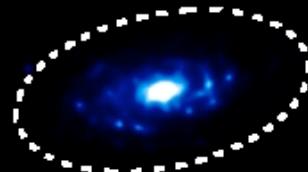


molecular
hydrogen

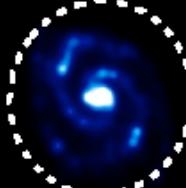
NGC 4736



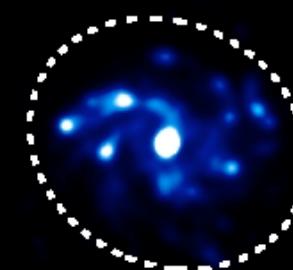
NGC 5055



NGC 5194

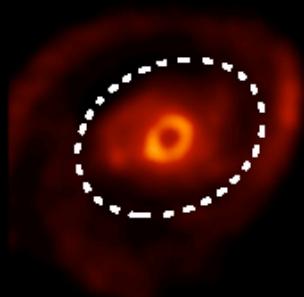


NGC 6946

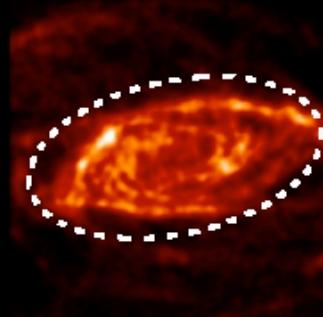


star
formation

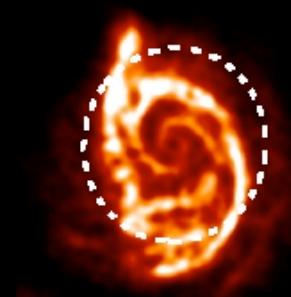
NGC 4736



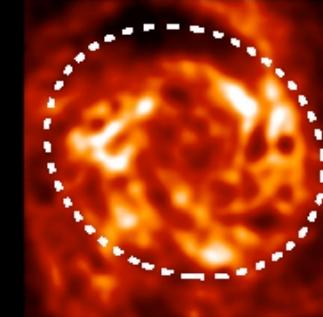
NGC 5055



NGC 5194

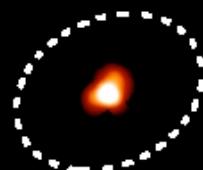


NGC 6946

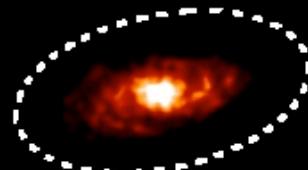


atomic
hydrogen

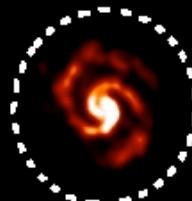
NGC 4736



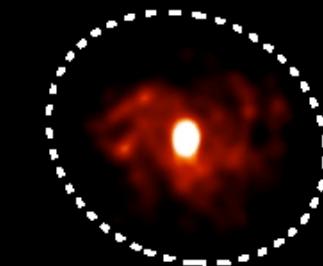
NGC 5055



NGC 5194



NGC 6946

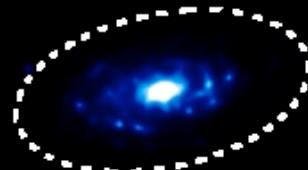


molecular
hydrogen

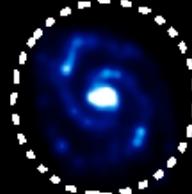
NGC 4736



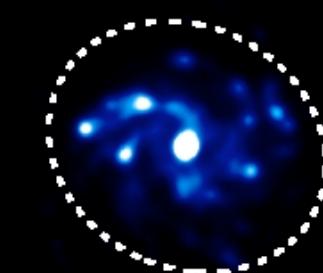
NGC 5055



NGC 5194

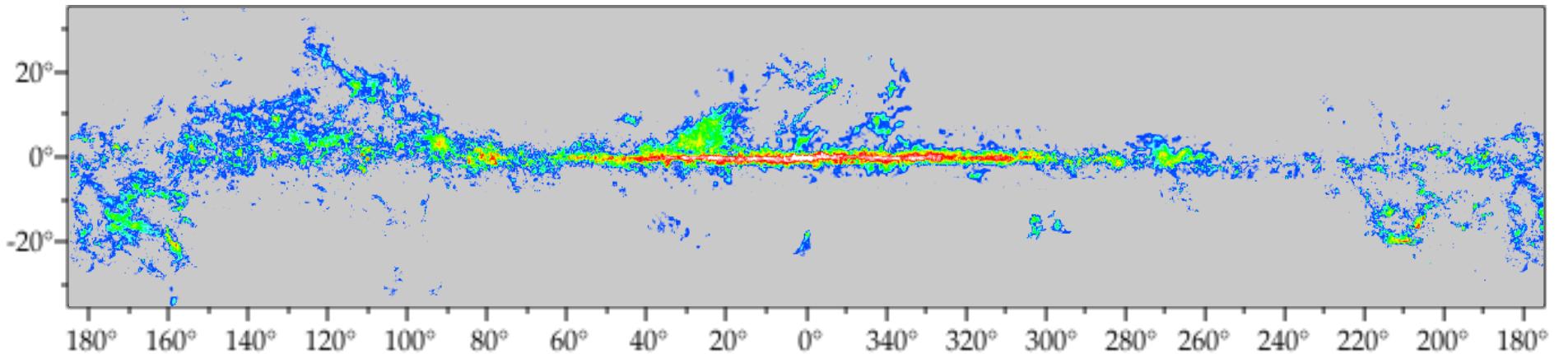


NGC 6946



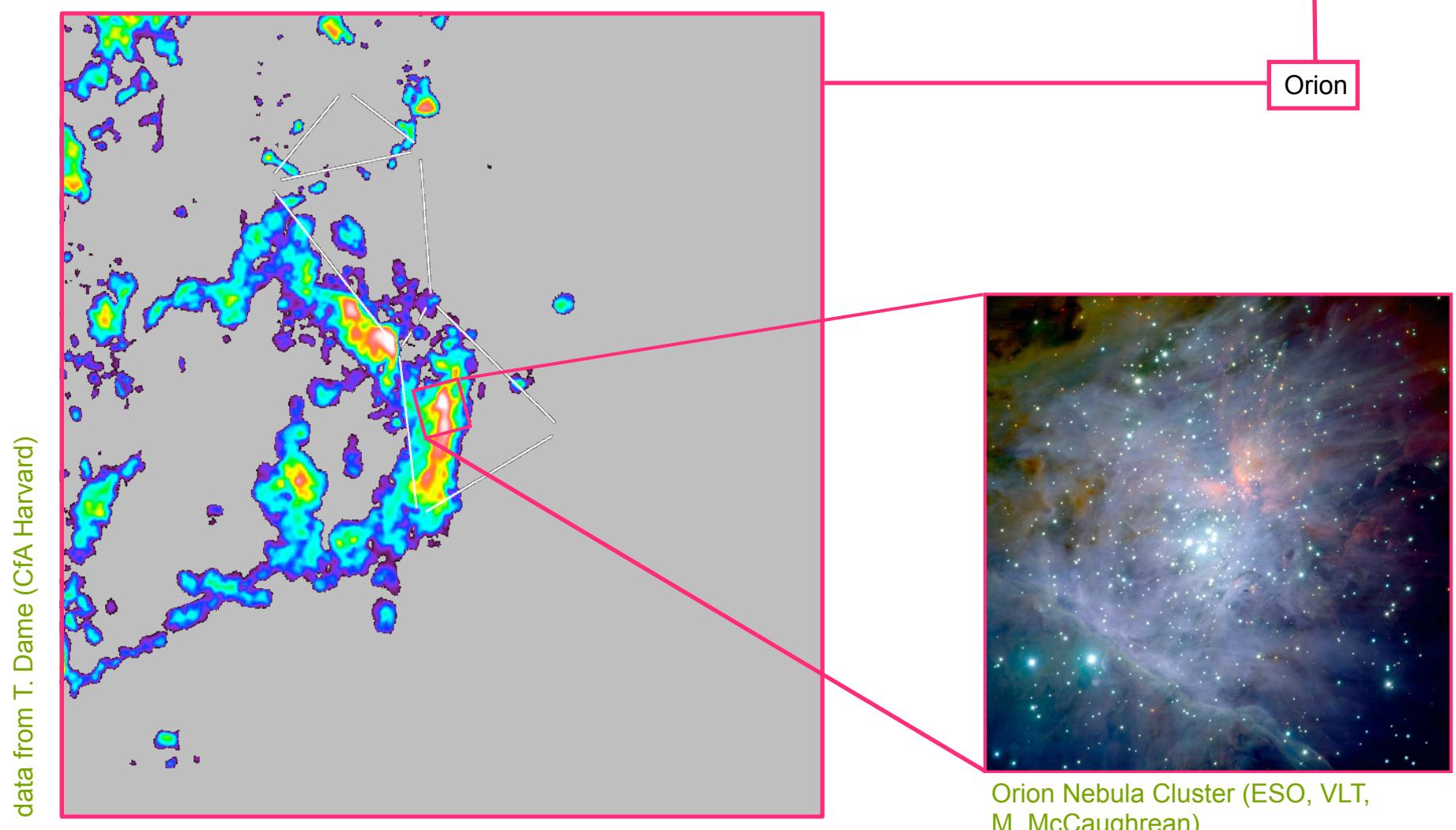
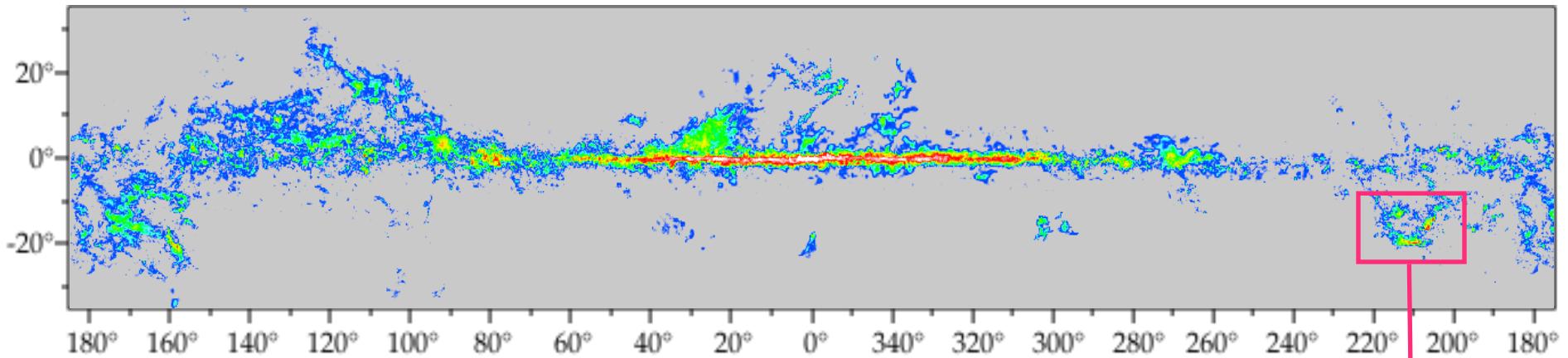
star
formation

- HI gas more extended
- H₂ and SF well correlated



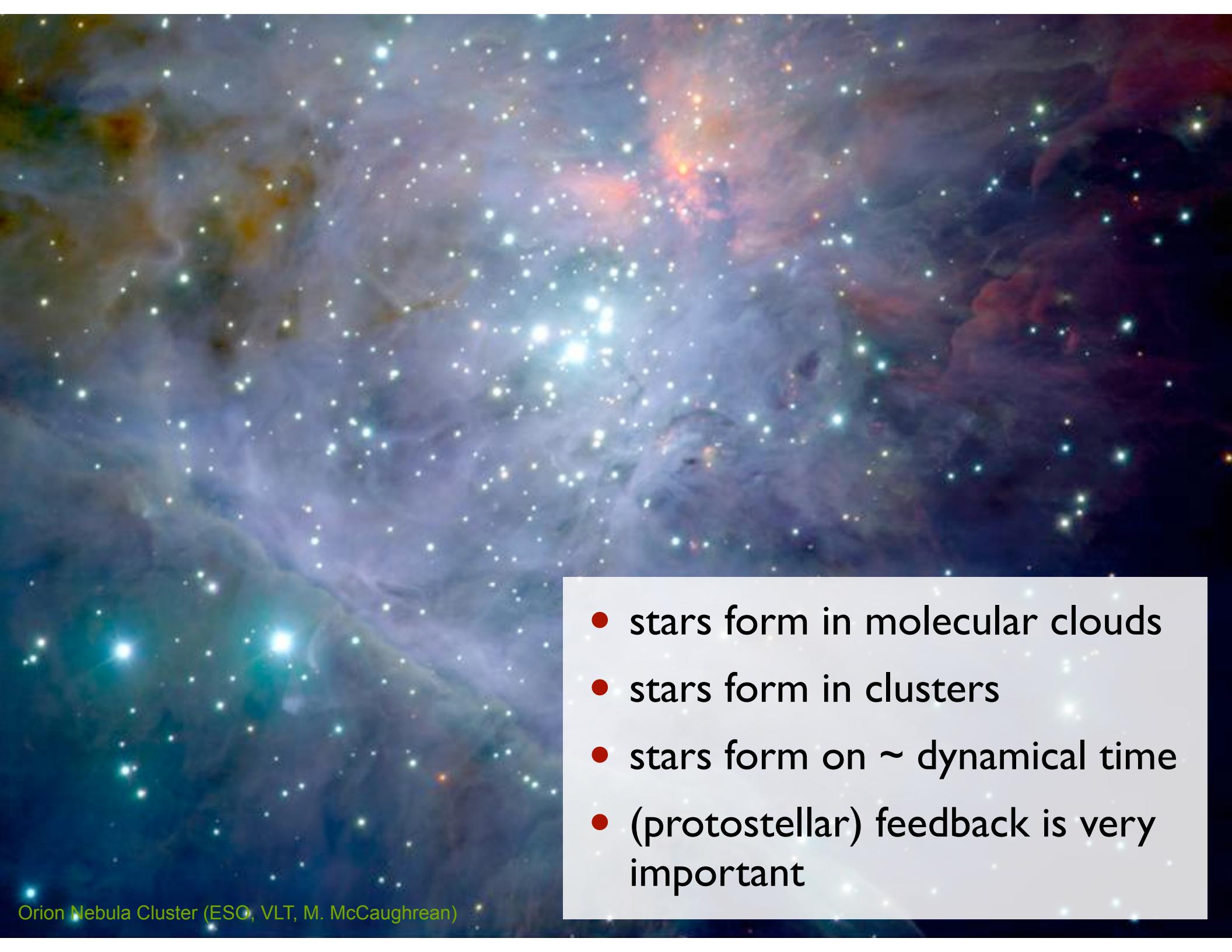
distribution of molecular
gas in the Milky Way as
traced by CO emission

data from T. Dame (CfA Harvard)



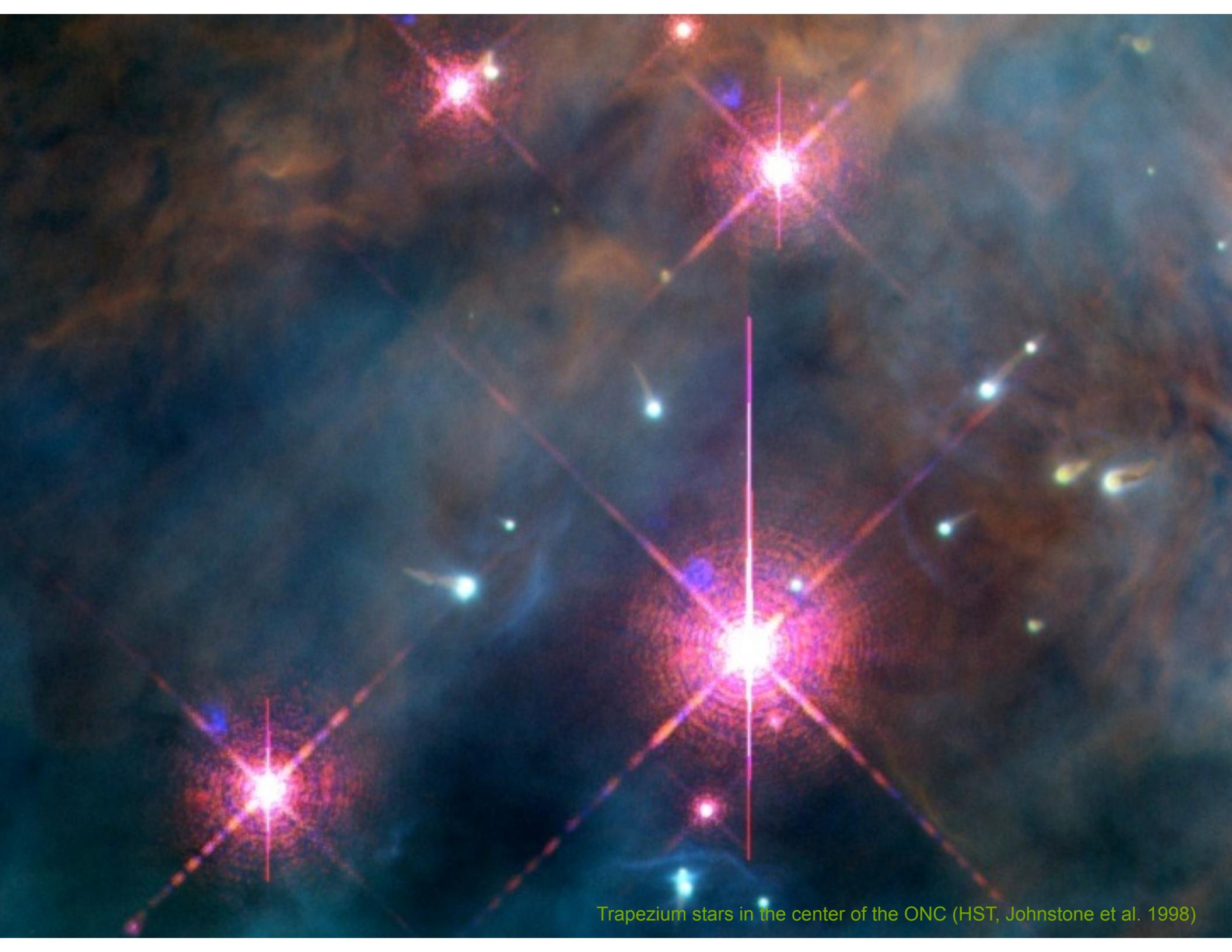


Orion Nebula Cluster (ESO, VLT, M. McCaughrean)



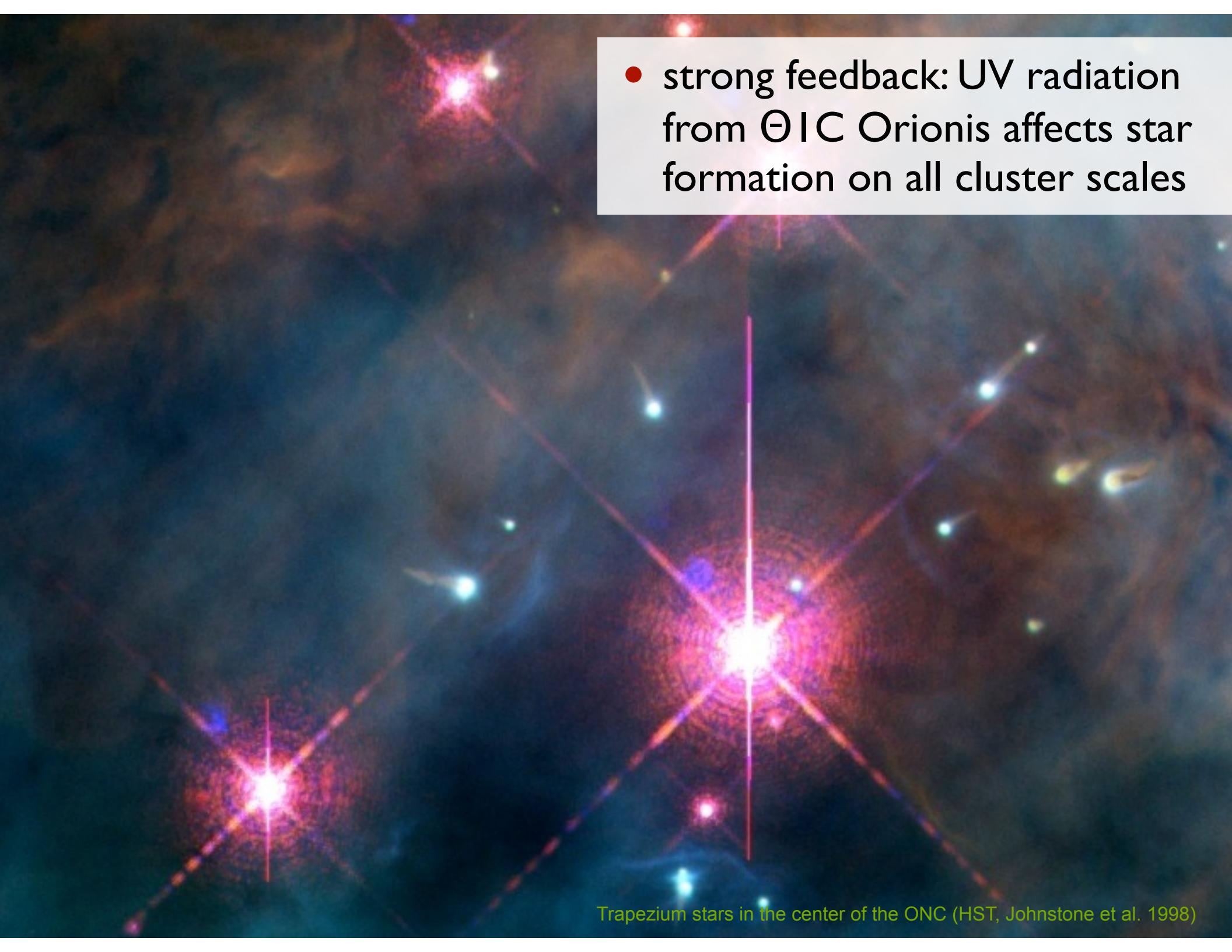
- stars form in molecular clouds
- stars form in clusters
- stars form on \sim dynamical time
- (protostellar) feedback is very important

Orion Nebula Cluster (ESO, VLT, M. McCaughrean)

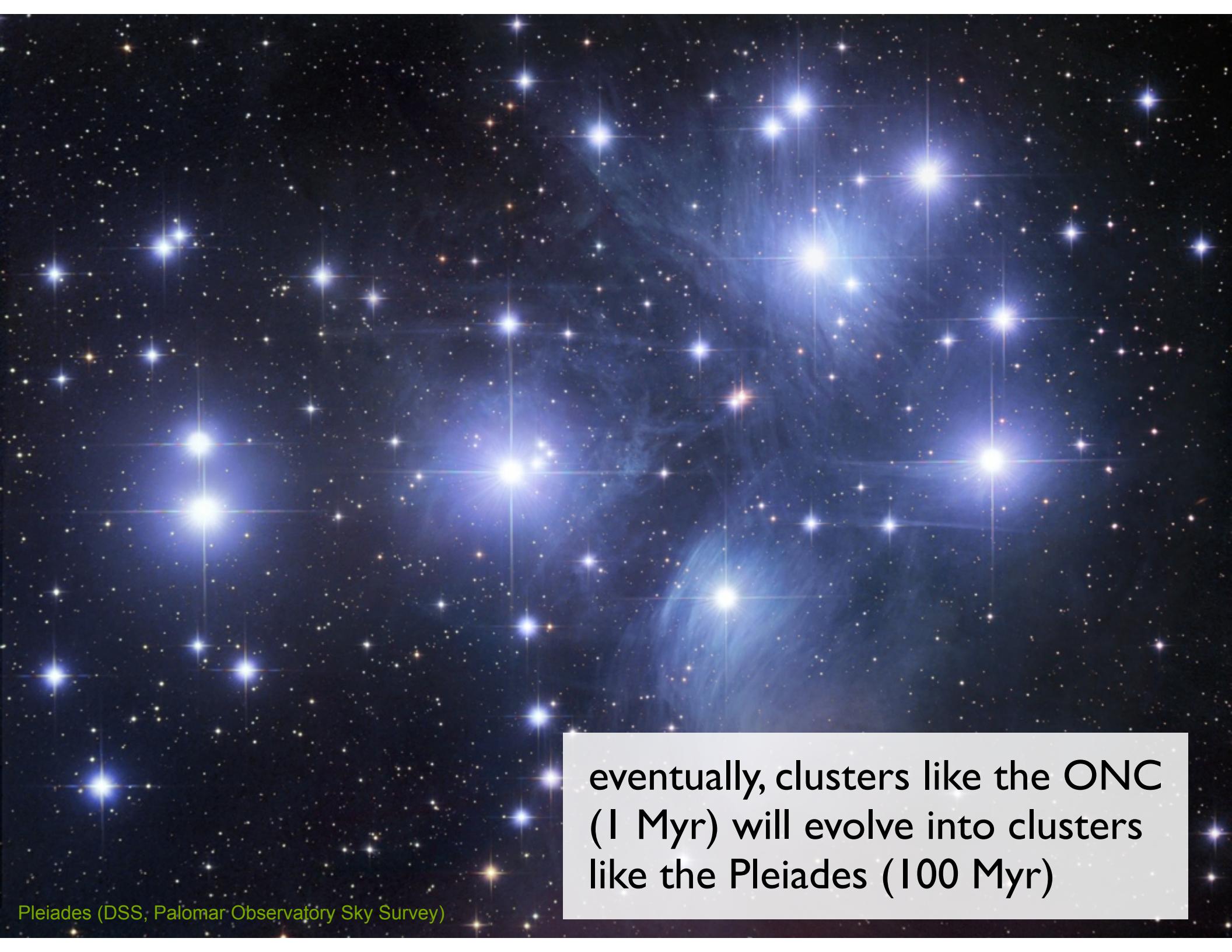


Trapezium stars in the center of the ONC (HST, Johnstone et al. 1998)

- strong feedback: UV radiation from Θ1C Orionis affects star formation on all cluster scales



Trapezium stars in the center of the ONC (HST, Johnstone et al. 1998)



eventually, clusters like the ONC
(1 Myr) will evolve into clusters
like the Pleiades (100 Myr)

theoretical
approach

decrease in spatial scale / increase in density



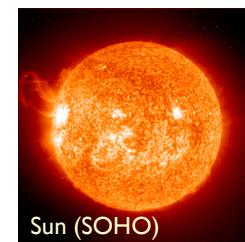
Andromeda (R. Gendler)



NGC 602 in LMC (Hubble)



Proplyd in Orion (Hubble)



Sun (SOHO)



Earth

- **density**
 - density of ISM: few particles per cm^3
 - density of molecular cloud: few 100 particles per cm^3
 - density of Sun: 1.4 g/ cm^3
- **spatial scale**
 - size of molecular cloud: few 10s of pc
 - size of young cluster: $\sim 1 \text{ pc}$
 - size of Sun: $1.4 \times 10^{10} \text{ cm}$

decrease in spatial scale / increase in density



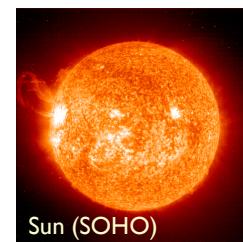
Andromeda (R. Gendler)



NGC 602 in LMC (Hubble)



Proplyd in Orion (Hubble)



Sun (SOHO)



Earth

- **contracting force**
 - only force that can do this compression is **GRAVITY**
- **opposing forces**
 - there are several processes that can oppose gravity
 - **GAS PRESSURE**
 - **TURBULENCE**
 - **MAGNETIC FIELDS**
 - **RADIATION PRESSURE**

decrease in spatial scale / increase in density



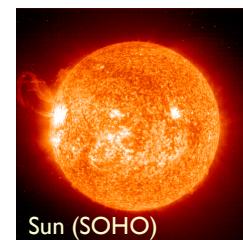
Andromeda (R. Gendler)



NGC 602 in LMC (Hubble)



Proplyd in Orion (Hubble)



Sun (SOHO)



Earth

- contracting force
 - only force that can do this compression is **GRAVITY**
- opposing forces
 - there are several processes that can oppose gravity
 - **GAS PRESSURE**
 - **TURBULENCE**
 - **MAGNETIC FIELDS**
 - **RADIATION PRESSURE**

Modern star formation theory is based on the complex interplay between *all* these processes.

early theoretical models

- *Jeans (1902)*: Interplay between self-gravity and thermal pressure

- stability of homogeneous spherical density enhancements against gravitational collapse
- dispersion relation:



Sir James Jeans, 1877 - 1946

$$\omega^2 = c_s^2 k^2 - 4\pi G \rho_0$$

- instability when $\omega^2 < 0$

- minimal mass: $M_J = \frac{1}{6} \pi^{-5/2} G^{-3/2} \rho_0^{-1/2} c_s^3 \propto \rho_0^{-1/2} T^{+3/2}$

first approach to turbulence

- von Weizsäcker (1943, 1951) and Chandrasekhar (1951): concept of **MICROTURBULENCE**

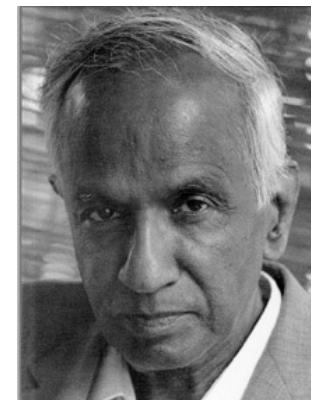
- BASIC ASSUMPTION: separation of scales between dynamics and turbulence

$$\ell_{\text{turb}} \ll \ell_{\text{dyn}}$$

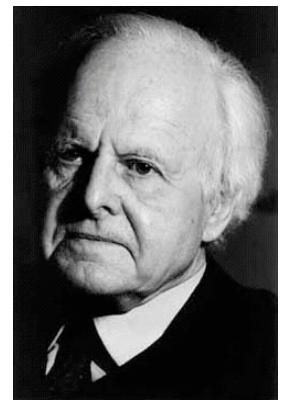
- then turbulent velocity dispersion contributes to effective soundspeed:

$$C_c^2 \mapsto C_c^2 + \sigma_{rms}^2$$

- → Larger effective Jeans masses → more stability
 - BUT: (1) *turbulence depends on k*: $\sigma_{rms}^2(k)$
(2) *supersonic turbulence* → $\sigma_{rms}^2(k) \gg C_s^2$ usually



S. Chandrasekhar,
1910 - 1995



C.F. von Weizsäcker,
1912 - 2007

problems of early dynamical theory

- molecular clouds are *highly Jeans-unstable*, yet, they do *NOT* form stars at high rate and with high efficiency (Zuckerman & Evans 1974 conundrum) (the observed global SFE in molecular clouds is $\sim 5\%$)
→ *something prevents large-scale collapse.*
- all throughout the early 1990's, molecular clouds had been thought to be long-lived quasi-equilibrium entities.
- molecular clouds are *magnetized*

magnetic star formation

- *Mestel & Spitzer (1956)*: Magnetic fields can prevent collapse!!!

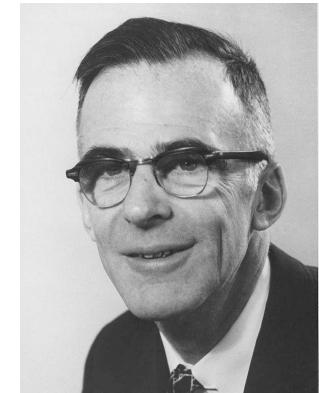
- Critical mass for gravitational collapse in presence of B-field

$$M_{cr} = \frac{5^{3/2}}{48\pi^2} \frac{B^3}{G^{3/2} \rho^2}$$

- Critical mass-to-flux ratio
(Mouschovias & Spitzer 1976)

$$\left[\frac{M}{\Phi} \right]_{cr} = \frac{\zeta}{3\pi} \left[\frac{5}{G} \right]^{1/2}$$

- Ambipolar diffusion can initiate collapse



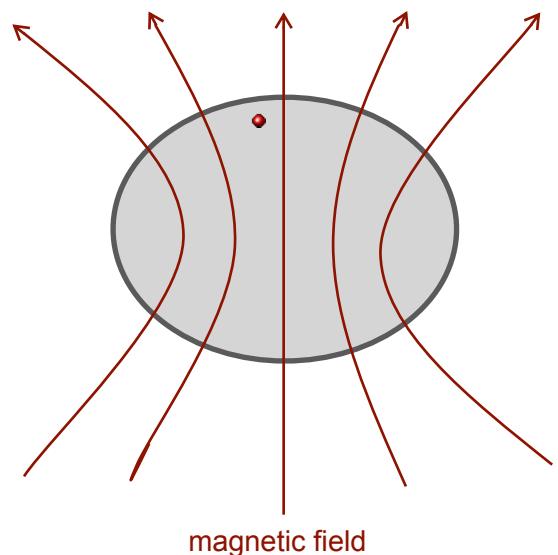
Lyman Spitzer, Jr., 1914 - 1997

“standard theory” of star formation

- BASIC ASSUMPTION: Stars form from magnetically highly subcritical cores
- Ambipolar diffusion slowly increases (M/Φ) : $\tau_{AD} \approx 10\tau_{ff}$
- Once $(M/\Phi) > (M/\Phi)_{crit}$: dynamical collapse of SIS
 - Shu (1977) collapse solution
 - $dM/dt = 0.975 c_s^3/G = \text{const.}$
- Was (in principle) only intended for isolated, low-mass stars



Frank Shu, 1943 -



problems of “standard theory”

- Observed B-fields are weak, at most marginally critical (Crutcher 1999, Bourke et al. 2001)
- Magnetic fields cannot prevent decay of turbulence
(Mac Low et al. 1998, Stone et al. 1998, Padoan & Nordlund 1999)
- Structure of prestellar cores
(e.g. Bacman et al. 2000, Alves et al. 2001)
- Strongly time varying dM/dt
(e.g. Hendriksen et al. 1997, André et al. 2000)
- More extended infall motions than predicted by the standard model
(Williams & Myers 2000, Myers et al. 2000)
- Most stars form as binaries
(e.g. Lada 2006)
- As many prestellar cores as protostellar cores in SF regions (e.g. André et al 2002)
- Molecular cloud clumps are chemically young
(Bergin & Langer 1997, Pratap et al 1997, Aikawa et al 2001)
- Stellar age distribution small ($\tau_{\text{ff}} \ll \tau_{\text{AD}}$)
(Ballesteros-Paredes et al. 1999, Elmegreen 2000, Hartmann 2001)
- Strong theoretical criticism of the SIS as starting condition for gravitational collapse
(e.g. Whitworth et al 1996, Nakano 1998, as summarized in Klessen & Mac Low 2004)
- Standard AD-dominated theory is incompatible with observations
(Crutcher et al. 2009, 2010ab, Bertram et al. 2011)

(see e.g. Mac Low & Klessen, 2004, Rev. Mod. Phys., 76, 125-194)

gravoturbulent star formation

- BASIC ASSUMPTION:

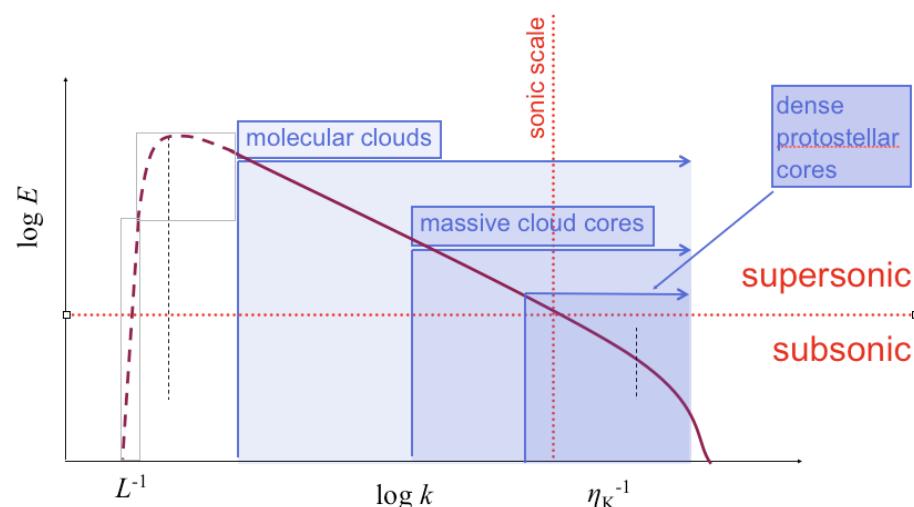
- star formation is controlled by interplay between supersonic turbulence and self-gravity

- turbulence plays a *dual role*:

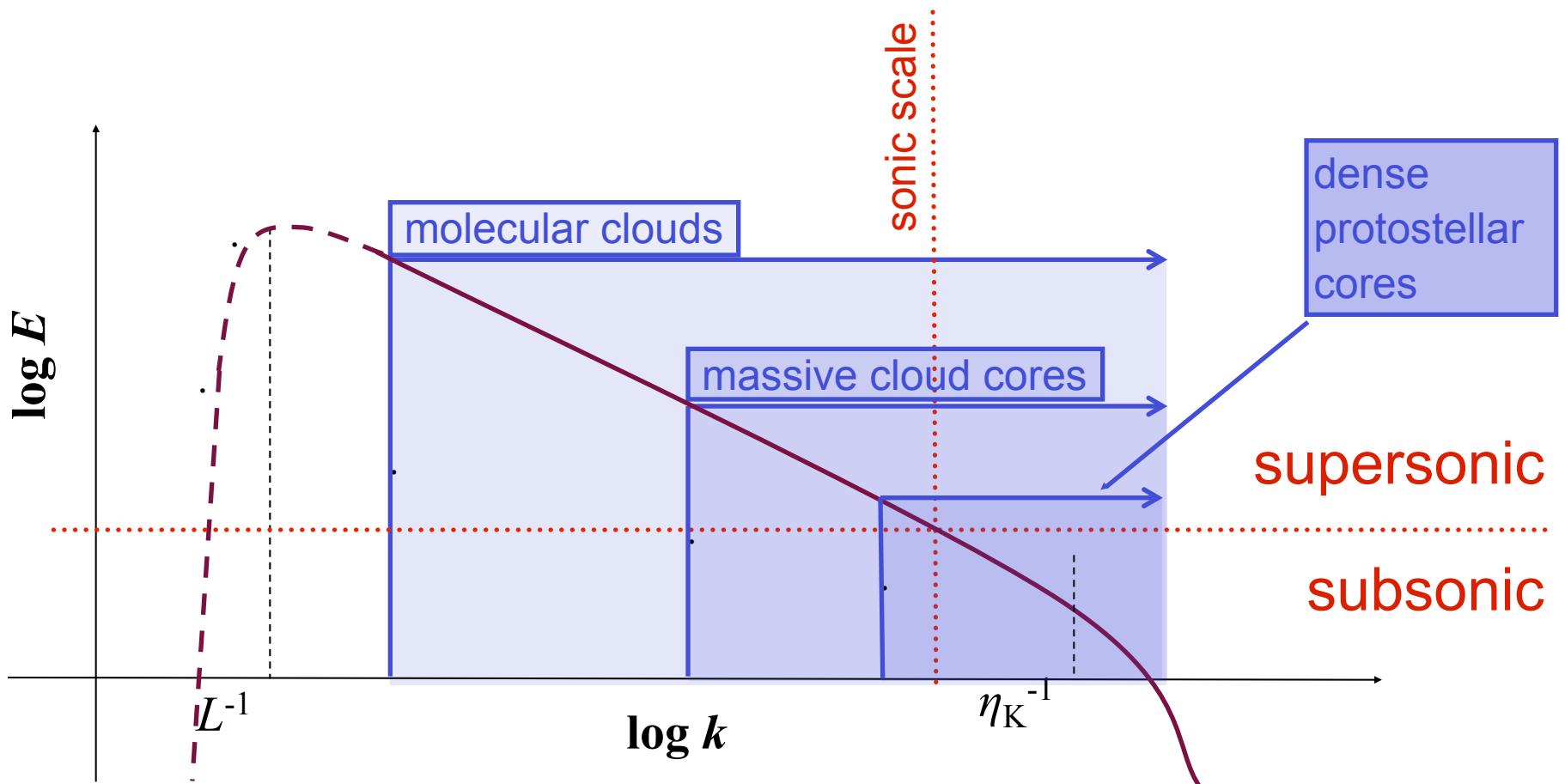
- on *large scales* it *provides support*
 - on *small scales* it can *trigger collapse*

- some predictions:

- dynamical star formation timescale τ_{ff}
 - high binary fraction
 - complex spatial structure of embedded star clusters
 - and many more . . .



turbulent cascade in the ISM



energy source & scale
NOT known
(supernovae, winds,
spiral density waves?)

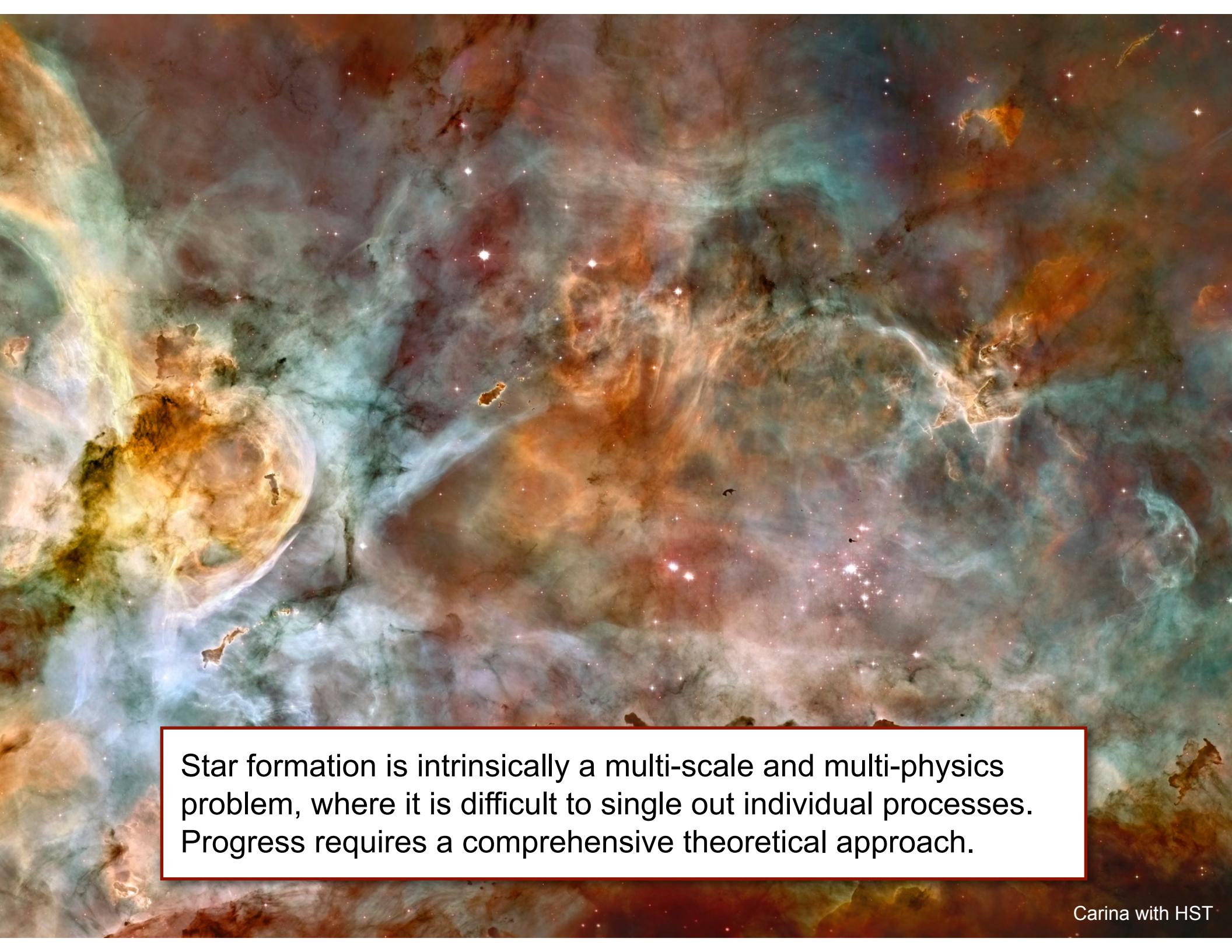
$\sigma_{\text{rms}} \ll 1 \text{ km/s}$
 $M_{\text{rms}} \leq 1$
 $L \approx 0.1 \text{ pc}$

dissipation scale not known
(ambipolar diffusion,
molecular diffusion?)

current status

- stars form from the complex interplay of self-gravity and a large number of competing processes (such as turbulence, magnetic fields, radiative and mechanical feedback, thermal pressure, cosmic rays, etc.)
- the relative importance of these processes depends on the environment
 - prestellar cores --> thermal pressure is important
 - molecular clouds --> turbulence dominates
 - massive star forming regions (NGC602): radiative feedback is important
 - small clusters (Taurus): evolution maybe dominated by external turbulence
- star formation is regulated by various feedback processes
- star formation is closely linked to global galactic dynamics (KS relation)

Star formation is intrinsically a multi-scale and multi-physics problem, where it is difficult to single out individual processes. Simple theoretical approaches usually fail.



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selected open questions

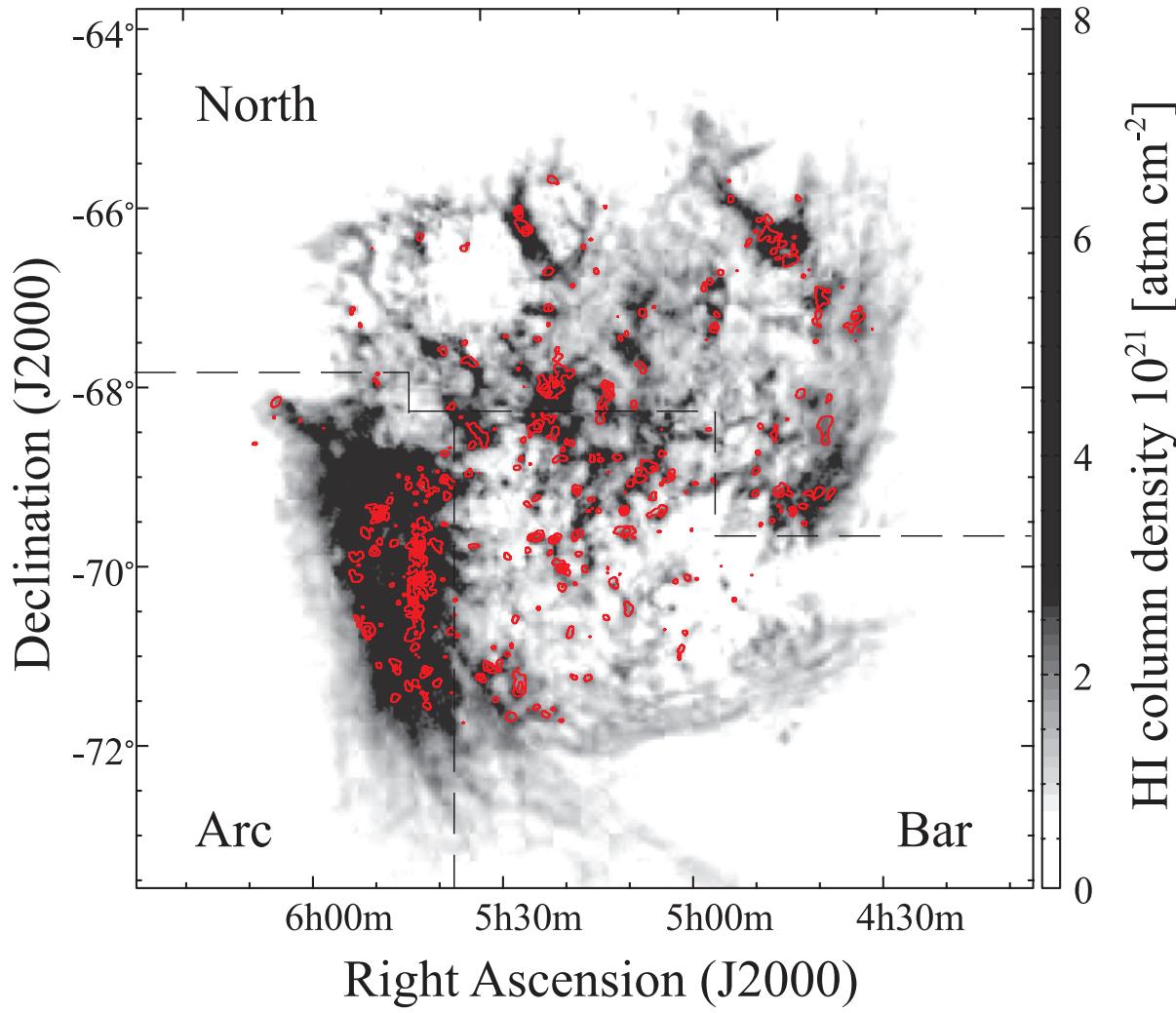
- what regulates star formation on galactic scales? global SF relations?
- what drives interstellar turbulence?
- how do molecular clouds form and evolve?
is there unaccounted (molecular) gas in galaxies?
- what are the initial conditions for star cluster formation?
how does cloud structure translate into cluster structure?
- what processes determine the initial mass function (IMF) of stars?
- how does star formation depend on metallicity? how do the first stars form?
- star formation in extreme environments (galactic center, starburst, etc.),
how does it differ from a more “normal” mode?

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molecular cloud
formation

molecular cloud formation

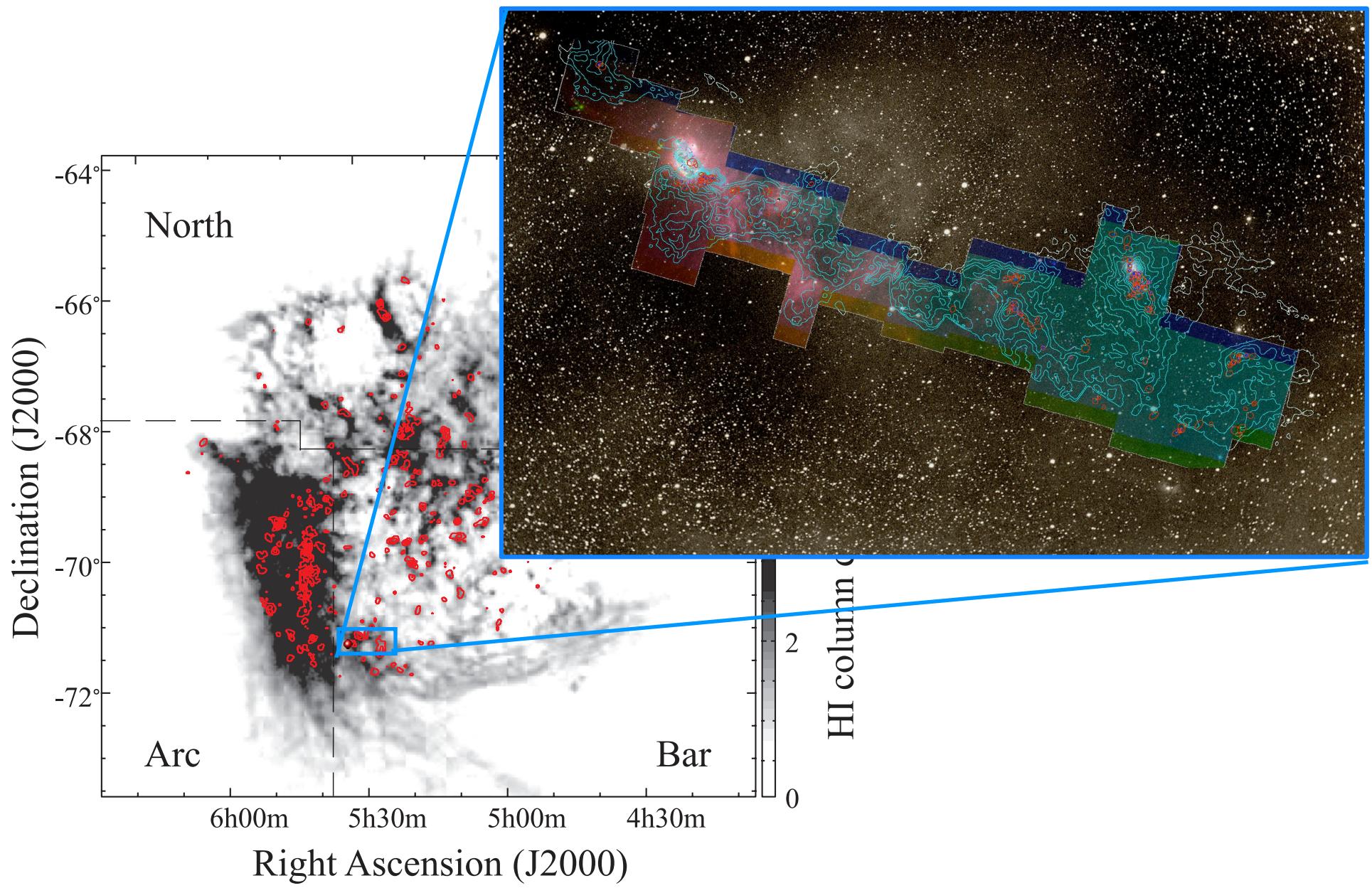


Idea:

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)

zooming in ...



position-position-velocity structure of the Perseus cloud

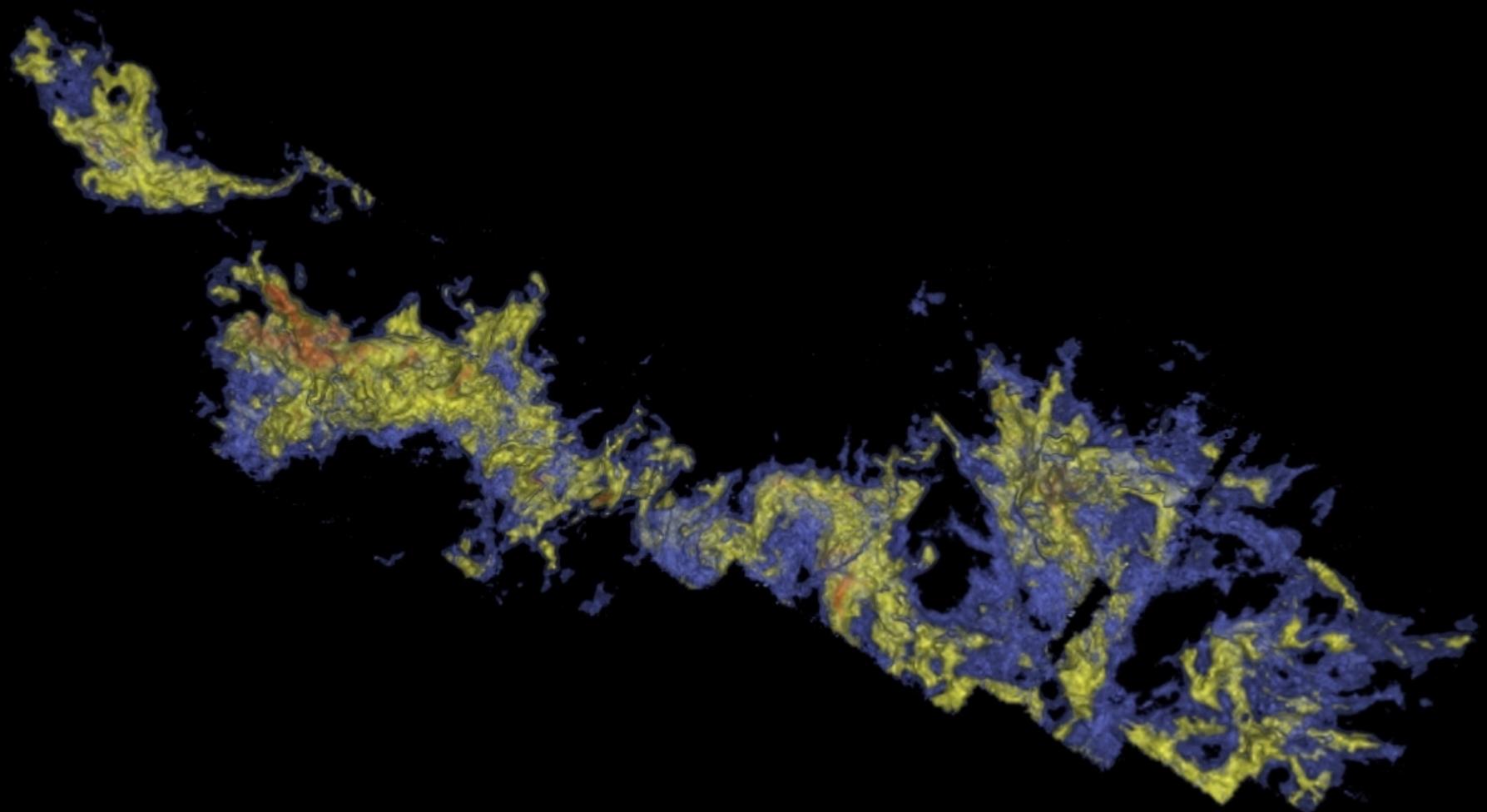
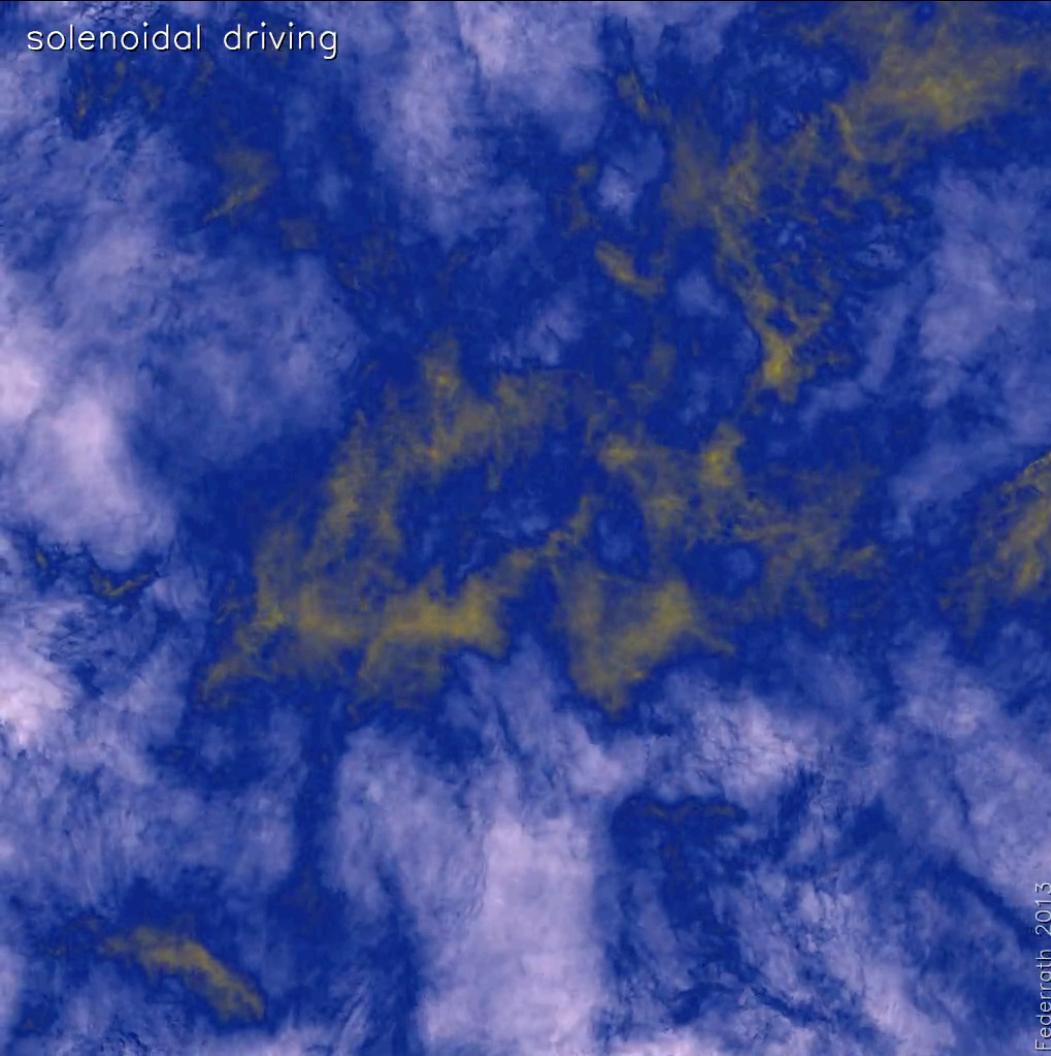


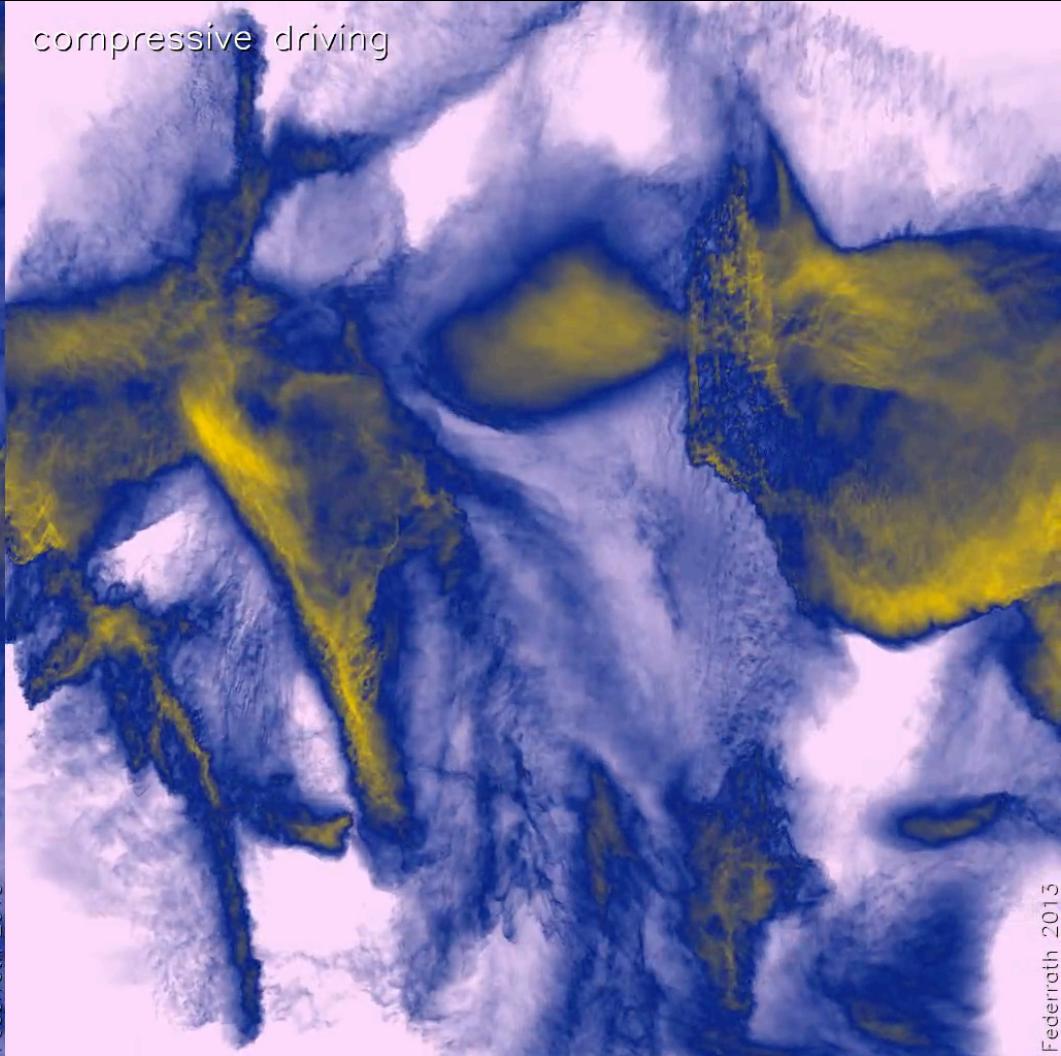
image from Alyssa Goodman: COMPLETE survey

density structure resulting from different turbulent driving schemes

solenoidal driving



compressive driving



driving with solenoidal modes

Federrath 2013

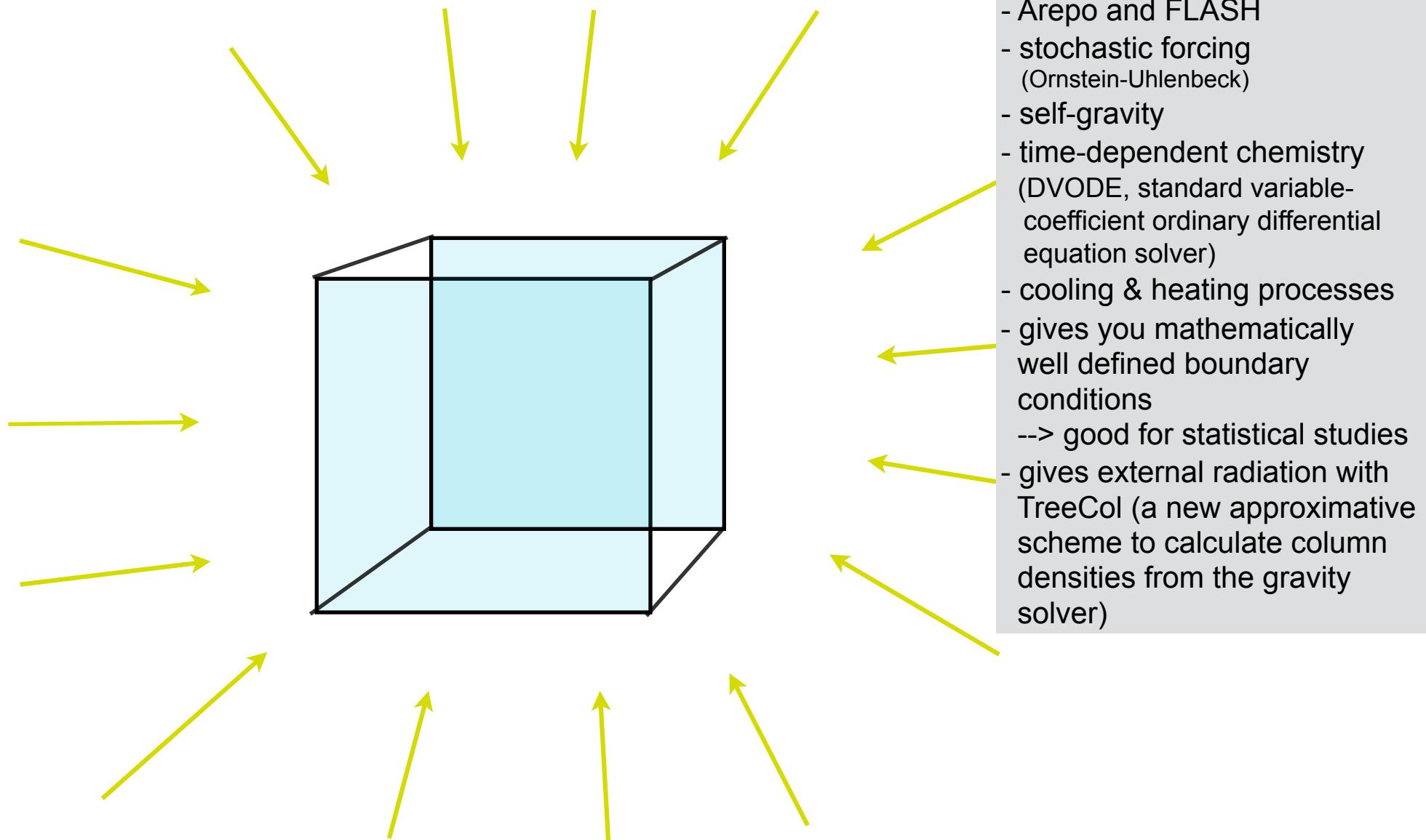
driving with compressive modes

(turbulent box of isothermal ideal gas)

Federrath 2013

including detailed
chemistry

experimental set-up



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



chemical model 1

Process

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

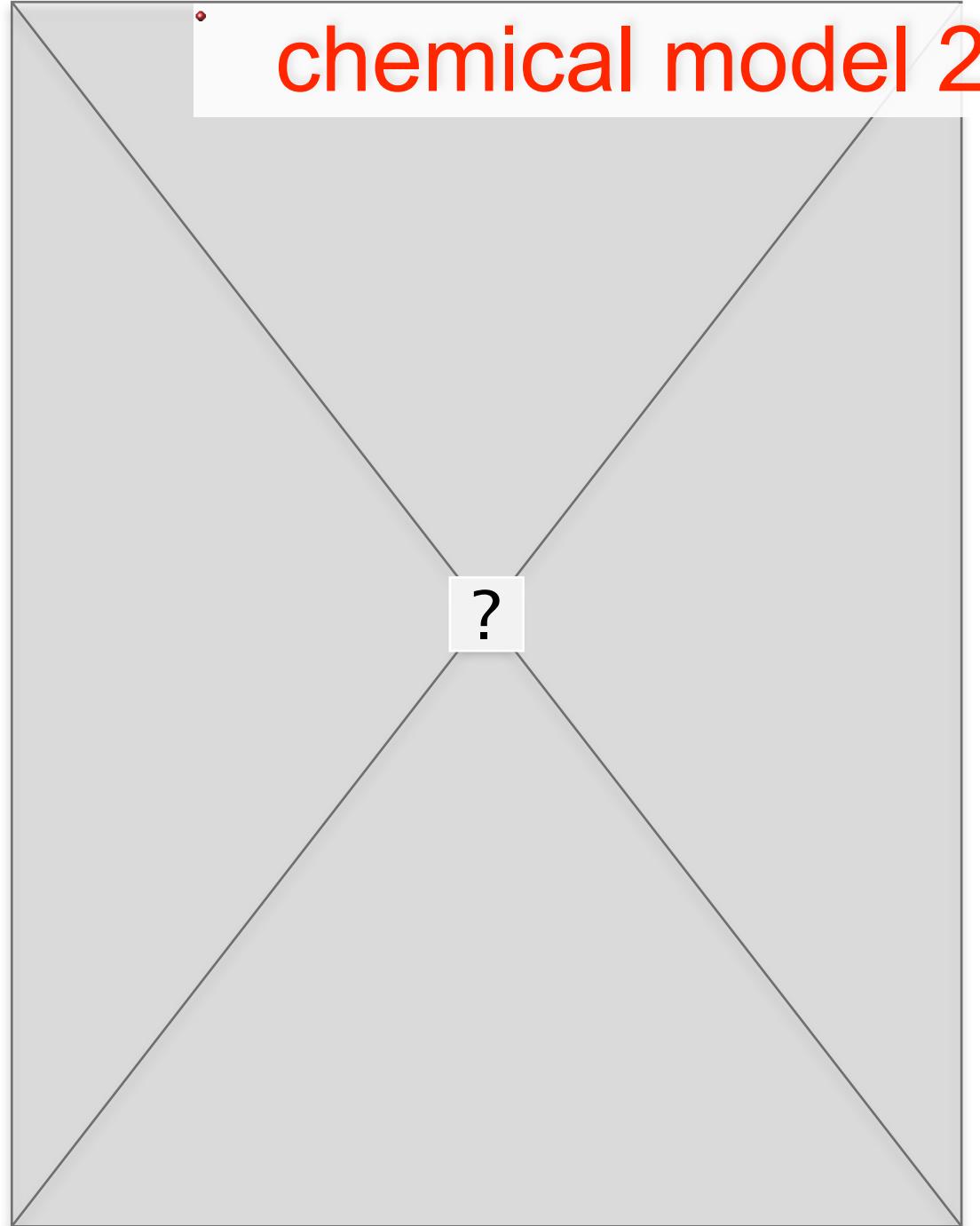
Burton, Hollenbach & Tielens (1990)

H_2 formation on dust grains

Hollenbach & McKee (1989)

Cosmic ray ionization

Goldsmith & Langer (1978)





14	$H^- + H \rightarrow H + H + e^-$	$k_{14} = 2.5634 \times 10^{-9} T_e^{1.78186}$ $= \exp[-2.0372609 \times 10^1$ $+ 1.13944933 \times 10^0 \ln T_e$ $- 1.4210135 \times 10^{-1} / (\ln T_e)^2$ $+ 8.4644554 \times 10^{-3} (\ln T_e)^3$ $- 3.1641 \times 10^{-3} (\ln T_e)^4$ $+ 2.1121 \times 10^{-4} (\ln T_e)^5$ $+ 8.6639632 \times 10^{-5} (\ln T_e)^6$ $- 2.5850097 \times 10^{-5} (\ln T_e)^7$ $+ 2.4555012 \times 10^{-6} (\ln T_e)^8$ $- 8.0683825 \times 10^{-8} (\ln T_e)^9]$	$T_e \lesssim 0.1 \text{ eV}$	13
15	$H^- + H^+ \rightarrow H_2^+ + e^-$	$k_{15} = 6.9 \times 10^{-9} T^{-0.35}$ $= 9.6 \times 10^{-7} T^{-0.90}$	$T_e > 0.1 \text{ eV}$ $T \lesssim 8000 \text{ K}$ $T > 8000 \text{ K}$	15
16	$He + e^- \rightarrow He^+ + e^- + e^-$	$k_{16} = \exp[-4.409864886 \times 10^1$ $+ 2.391596563 \times 10^1 \ln T_e$ $- 1.07532302 \times 10^1 (\ln T_e)^2$ $+ 3.05803875 \times 10^0 (\ln T_e)^3$ $- 5.6851189 \times 10^{-1} (\ln T_e)^4$ $+ 6.79539123 \times 10^{-2} (\ln T_e)^5$ $- 5.0090561 \times 10^{-3} (\ln T_e)^6$ $+ 2.06723616 \times 10^{-4} (\ln T_e)^7$ $- 3.64916141 \times 10^{-6} (\ln T_e)^8]$		13
17	$He^+ + e^- \rightarrow He + \gamma$	$k_{17,rr,A} = 10^{-11} T^{-0.5} [12.72 - 1.615 \log T$ $- 0.3162(\log T)^2 + 0.0493(\log T)^3]$ $k_{17,rr,B} = 10^{-11} T^{-0.5} [11.19 - 1.676 \log T$ $- 0.2852(\log T)^2 + 0.04433(\log T)^3]$ $k_{17,di} = 1.9 \times 10^{-3} T^{-1.5} \exp\left(-\frac{473421}{T}\right)$ $\times [1.0 + 0.3 \exp\left(-\frac{94684}{T}\right)]$	Case A Case B	16 16
18	$He^+ + H \rightarrow He + H^+$	$k_{18} = 1.25 \times 10^{-15} \left(\frac{T}{300}\right)^{0.25}$		17
19	$He + H^+ \rightarrow He^+ + H$	$k_{19} = 1.26 \times 10^{-9} T^{-0.75} \exp\left(-\frac{127500}{T}\right)$ $= 4.0 \times 10^{-37} T^{4.74}$	$T \lesssim 10000 \text{ K}$ $T > 10000 \text{ K}$	18 19
20	$C^+ + e^- \rightarrow C + \gamma$	$k_{20} = 4.67 \times 10^{-12} \left(\frac{T}{300}\right)^{-0.6}$ $= 1.23 \times 10^{-17} \left(\frac{T}{300}\right)^{2.49} \exp\left(\frac{21845.6}{T}\right)$ $= 9.62 \times 10^{-8} \left(\frac{T}{300}\right)^{-1.37} \exp\left(-\frac{115786.2}{T}\right)$	$T \lesssim 7950 \text{ K}$ $7950 \text{ K} < T \lesssim 21140 \text{ K}$ $T > 21140 \text{ K}$	20
21	$O^+ + e^- \rightarrow O + \gamma$	$k_{21} = 1.30 \times 10^{-10} T^{-0.64}$ $= 4.11 \times 10^{-10} T^{-0.66} + 7.4 \times 10^{-4} T^{-1.5}$ $\times \exp\left(-\frac{175000}{T}\right) [1.0 + 0.062 \times \exp\left(-\frac{145000}{T}\right)]$	$T \lesssim 400 \text{ K}$ $T > 400 \text{ K}$	21 22
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	$O + H^+ \rightarrow O^+ + H$	$k_{25} = [1.08 \times 10^{-11} T^{0.517}$ $+ 4.00 \times 10^{-10} T^{0.00669}] \exp\left(-\frac{227}{T}\right)$		24
26	$O + He^+ \rightarrow O^+ + He$	$k_{26} = 4.991 \times 10^{-15} \left(\frac{T}{10000}\right)^{0.3794} \exp\left(-\frac{T}{1121000}\right)$ $+ 2.780 \times 10^{-15} \left(\frac{T}{10000}\right)^{-0.2163} \exp\left(\frac{T}{815800}\right)$		25
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	$C + He^+ \rightarrow C^+ + He$	$k_{29} = 8.58 \times 10^{-17} T^{0.757}$ $= 3.25 \times 10^{-17} T^{0.968}$ $= 2.77 \times 10^{-19} T^{1.597}$	$T \lesssim 200 \text{ K}$ $200 < T \lesssim 2000 \text{ K}$ $T > 2000 \text{ K}$	26
30	$H_2 + He \rightarrow H + H + He$	$k_{30,i} = \text{dex} [-27.029 + 3.801 \log(T) - 29487/T]$ $k_{30,h} = \text{dex} [-2.729 - 1.75 \log(T) - 23474/T]$ $n_{cr,He} = \text{dex} [5.0792(1.0 - 1.23 \times 10^{-5}(T - 2000))]$		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



14	$H^- + H \rightarrow H + H + e^-$	$k_{14} = 2.5634 \times 10^{-9} T_e^{1.78186}$	$T_e \leq 0.1 \text{ eV}$	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	$CH + C \rightarrow CO + H$	$k_{38} = 6.6 \times 10^{-11}$ $= 1.09 \times 10^{-10} \exp\left(-\frac{14}{T}\right)$	$T \leq 2000 \text{ K}$ $T > 2000 \text{ K}$	35 36
39	$CO + H \rightarrow CH_2 + H$	$k_{39} = 2.0 \times 10^{-11}$		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	$C_2 + O \rightarrow CO + C$	$k_{42} = 5.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.5}$ $= 5.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.757}$	$T \leq 300 \text{ K}$ $T > 300 \text{ K}$	40 41
15	H^-			
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
16	He^-			
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	$OH + O \rightarrow O_2 + H$	$k_{47} = 3.50 \times 10^{-11}$ $= 1.77 \times 10^{-11} \exp\left(\frac{178}{T}\right)$	$T \leq 261 \text{ K}$ $T > 261 \text{ K}$	45 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
17	He^+			
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	$O_2 + C \rightarrow CO + O$	$k_{52} = 4.7 \times 10^{-11} \left(\frac{T}{300}\right)^{-0.34}$ $= 2.48 \times 10^{-12} \left(\frac{T}{300}\right)^{1.54} \exp\left(\frac{613}{T}\right)$	$T \leq 295 \text{ K}$ $T > 295 \text{ K}$	34 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
18	He^{+}			
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
19	He^{+}			
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
20	C^+			
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
21	O^+			
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
22	C_+			
64	$CH_2^+ + H_2 \rightarrow CH_3^+ + H$	$k_{64} = 1.6 \times 10^{-9}$		53
23	O_+			
65	$CH_2^+ + O \rightarrow HCO^+ + H$	$k_{65} = 7.5 \times 10^{-10}$		28
24	O_+			
66	$CH_3^+ + H \rightarrow CH_2^+ + H_2$	$k_{66} = 7.0 \times 10^{-10} \exp\left(-\frac{10560}{T}\right)$		28
25	O_+			
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
26	O_+			
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
27	C_+			
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
28	C^+			
73	$OH + C^+ \rightarrow CO^+ + H$	$k_{73} = 7.7 \times 10^{-10}$		28
29	C_+			
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
30	H_2			
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
31	OH			
80	$O_2 + C^+ \rightarrow CO^+ + O$	$k_{80} = 3.8 \times 10^{-10}$		53
32	HO			
81	$O_2 + C^+ \rightarrow CO + O^+$	$k_{81} = 6.2 \times 10^{-10}$		53
33	HO			
82	$O_2 + CH_2^+ \rightarrow HCO^+ + OH$	$k_{82} = 9.1 \times 10^{-10}$		53
34	C_+			
83	$O_2^+ + C \rightarrow CO^+ + O$	$k_{83} = 5.2 \times 10^{-11}$		28
35	CH			
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



chemical model 2

14	$H^- + H \rightarrow H + H + e^-$	88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$	63		
	$36 CH + H_2^- \rightarrow$	89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{T}{T_c}\right)$	63		
	$37 CH + C^- \rightarrow$	90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$	28		
	$38 CH + C^- \rightarrow$	91	$CH_2 + H^+ \rightarrow CH_2^+ + H$	$k_{91} = 1.4 \times 10^{-9}$	28		
	$92 CH_2 + H^+ \rightarrow C_2^+ + e^- + H_2$	92	$C_2^+ + H^+ \rightarrow C_2^+ + e^- + H_2$	$k_{92} = 5.0 \times 10^{-11}$	28		
	$39 C_2 + H^+ \rightarrow$	93	$C_2^+ + e^- \rightarrow C_2^+ + e^- + H_2$	93	28		
	$40 CH_2 + O^- \rightarrow$	94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-9}$	28		
	$41 CH_2 + O^- \rightarrow$	95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$	28		
	$42 C_2 + O^- \rightarrow$	96	$H_2O + H^+ \rightarrow H_2O^+ + H$	$k_{96} = 6.9 \times 10^{-9}$	64		
	$97 H_2O + He^+ \rightarrow OH + He + H^+$	97	$H_2O + He^+ \rightarrow OH + He + H^+$	$k_{97} = 2.04 \times 10^{-10}$	65		
15	H^-	98	$H_2O + He^+ \rightarrow OH^+ + He + H$	$k_{98} = 2.86 \times 10^{-10}$	65		
16	He^-	43	$O + H_2 \rightarrow$	99	$H_2O + He^+ \rightarrow H_2O^+ + He$	$k_{99} = 6.05 \times 10^{-11}$	65
	$44 OH + H \rightarrow$	100	$O_2 + H^+ \rightarrow O_2^+ + H$	$k_{100} = 2.0 \times 10^{-9}$	64		
	$45 OH + H_2 \rightarrow$	101	$O_2 + He^+ \rightarrow O_2^+ + He$	$k_{101} = 3.3 \times 10^{-11}$	66		
	$46 OH + C \rightarrow$	102	$O_2 + He^+ \rightarrow O^+ + O + He$	$k_{102} = 1.1 \times 10^{-9}$	66		
	$47 OH + O^- \rightarrow$	103	$O_2^+ + C \rightarrow O_2 + C^+$	$k_{103} = 5.2 \times 10^{-11}$	28		
	$104 CO + He^+ \rightarrow C^+ + O + He$	104	$CO + He^+ \rightarrow C^+ + O + He$	$k_{104} = 1.4 \times 10^{-9} \left(\frac{T}{300}\right)^{-0.5}$	67		
	$105 CO + He^+ \rightarrow C + O^+ + He$	105	$CO + He^+ \rightarrow C + O^+ + He$	$k_{105} = 1.4 \times 10^{-16} \left(\frac{T}{300}\right)^{-0.5}$	67		
	$106 CO^+ + H \rightarrow CO + H^+$	106	$CO^+ + H \rightarrow CO + H^+$	$k_{106} = 7.5 \times 10^{-10}$	68		
	$107 C^- + H^+ \rightarrow C + H$	107	$C^- + H^+ \rightarrow C + H$	$k_{107} = 2.3 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	28		
17	He^+	50	$O_2 + H \rightarrow$	108	$O^- + H^+ \rightarrow O + H$	$k_{108} = 2.3 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	28
	$51 O_2 + H_2 \rightarrow$	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		
	$52 O_2 + C \rightarrow$	110	$H_3^+ + e^- \rightarrow H_2 + H$	$k_{110} = 2.34 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.52}$	70		
	$111 H_3^+ + e^- \rightarrow H + H + H$	111	$H_3^+ + e^- \rightarrow H + H + H$	$k_{111} = 4.36 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.52}$	70		
	$53 CO + H \rightarrow$	112	$CH^+ + e^- \rightarrow C + H$	$k_{112} = 7.0 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	71		
18	He^+	54	$H_2^+ + H_2 \rightarrow$	113	$CH_2^+ + e^- \rightarrow CH + H$	$k_{113} = 1.6 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.6}$	72
	$55 H_3^+ + H \rightarrow$	114	$CH_2^+ + e^- \rightarrow C + H + H$	$k_{114} = 4.03 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.6}$	72		
	$56 C + H_2^+ \rightarrow$	115	$CH_2^+ + e^- \rightarrow C + H_2$	$k_{115} = 7.68 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.6}$	72		
19	He^+	57	$C + H_3^+ \rightarrow$	116	$CH_3^+ + e^- \rightarrow CH_2 + H$	$k_{116} = 7.75 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	73
	$58 C^+ + H_2 \rightarrow$	117	$CH_3^+ + e^- \rightarrow CH + H_2$	$k_{117} = 1.95 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	73		
	$59 CH^+ + H \rightarrow$	118	$CH_3^+ + e^- \rightarrow CH + H + H$	$k_{118} = 2.0 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.4}$	28		
	$60 CH^+ + H_2 \rightarrow$	119	$OH^+ + e^- \rightarrow O + H$	$k_{119} = 6.3 \times 10^{-9} \left(\frac{T}{300}\right)^{-0.48}$	74		
	$61 CH^+ + O \rightarrow$	120	$H_2O^+ + e^- \rightarrow O + H + H$	$k_{120} = 3.05 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	75		
20	C^+	62	$CH_2 + H^+ \rightarrow$	121	$H_2O^+ + e^- \rightarrow O + H_2$	$k_{121} = 3.9 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	75
	$63 CH_2^+ + H \rightarrow$	122	$H_2O^+ + e^- \rightarrow OH + H$	$k_{122} = 8.6 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	75		
	$64 CH_2^+ + H_2 \rightarrow$	123	$H_3O^+ + e^- \rightarrow H + H_2O$	$k_{123} = 1.08 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	76		
	$65 CH_2^+ + O \rightarrow$	124	$H_3O^+ + e^- \rightarrow OH + H_2$	$k_{124} = 6.02 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	76		
	$66 CH_3^+ + H \rightarrow$	125	$H_3O^+ + e^- \rightarrow OH + H + H$	$k_{125} = 2.58 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	76		
	$67 CH_3^+ + O \rightarrow$	126	$H_3O^+ + e^- \rightarrow O + H + H_2$	$k_{126} = 5.6 \times 10^{-9} \left(\frac{T}{300}\right)^{-0.5}$	76		
	$68 C_2 + O^+ \rightarrow$	127	$O_2^+ + e^- \rightarrow O + O$	$k_{127} = 1.95 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.7}$	77		
	$69 O^+ + H_2 \rightarrow$	128	$CO^+ + e^- \rightarrow C + O$	$k_{128} = 2.75 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.55}$	78		
	$70 O + H_2^+ \rightarrow$	129	$HCO^+ + e^- \rightarrow CO + H$	$k_{129} = 2.76 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.64}$	79		
27	C^+	71	$O + H_3^+ \rightarrow$	130	$HCO^+ + e^- \rightarrow OH + C$	$k_{130} = 2.4 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.64}$	79
	$72 OH + H_3^+ \rightarrow$	131	$HOC^+ + e^- \rightarrow CO + H$	$k_{131} = 1.1 \times 10^{-7} \left(\frac{T}{300}\right)^{-1.0}$	28		
	$73 OH + C^+ \rightarrow$	132	$H^- + C \rightarrow CH + e^-$	$k_{132} = 1.0 \times 10^{-9}$	28		
	$74 OH^+ + H_2 \rightarrow$	133	$H^- + O \rightarrow OH + e^-$	$k_{133} = 1.0 \times 10^{-9}$	28		
	$75 H_2O^+ + H \rightarrow$	134	$H^- + OH \rightarrow H_2O + e^-$	$k_{134} = 1.0 \times 10^{-10}$	28		
30	H_2	76	$H_2O + H_3^+ \rightarrow$	135	$C^- + H \rightarrow CH + e^-$	$k_{135} = 5.0 \times 10^{-10}$	28
	$77 H_2O + C^+ \rightarrow$	136	$C^- + H_2 \rightarrow CH_2 + e^-$	$k_{136} = 1.0 \times 10^{-13}$	28		
	$78 H_2O + C^+ \rightarrow$	137	$C^- + O \rightarrow CO + e^-$	$k_{137} = 5.0 \times 10^{-10}$	28		
	$79 H_3O^+ + C \rightarrow$	138	$O^- + H \rightarrow OH + e^-$	$k_{138} = 5.0 \times 10^{-10}$	28		
	$80 O_2 + C^+ \rightarrow$	139	$O^- + H_2 \rightarrow H_2O + e^-$	$k_{139} = 7.0 \times 10^{-10}$	28		
	$81 O_2 + C^+ \rightarrow$	140	$O^- + C \rightarrow CO + e^-$	$k_{140} = 5.0 \times 10^{-10}$	28		
	$82 O_2 + CH_2^+ \rightarrow$	87	$HCO^+ + H_2O \rightarrow CO + H_3O^+$	$k_{87} = 2.5 \times 10^{-9}$	28		



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14	$H^- + H \rightarrow H + H + e^-$	88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$	63	
	$CH + H_2 \rightarrow$	89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{T}{T_d}\right)$	63	
	$CH + C \rightarrow$	90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$	28	
	$CH + O \rightarrow$	91	$CH_2 + H^+ \rightarrow CH_2^+ + H$	$k_{91} = 1.4 \times 10^{-9}$	28	
	$CH_2 + H^+ \rightarrow C^+ + e^- + H_2$	92		$\approx 1.2 \times 10^{-11}$	28	
	$C + H_2 \rightarrow$	93	$C_2 + H^+ \rightarrow C + C^+ + e^-$	$\approx 0.6 \times 10^{-9}$	28	
	$CH_2 + O \rightarrow$	94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-9}$	28	
	$CH_2 + O \rightarrow$	95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$	28	
	$H_2O + H^+ \rightarrow H_2O^+ + H$	96		$k_{96} = 6.9 \times 10^{-9}$	64	
	$C_2 + O \rightarrow$	97	$H_2O + He^+ \rightarrow OH + He + H^+$	$k_{97} = 2.04 \times 10^{-10}$	65	
		98		$\approx 0.2 \times 10^{-10}$	65	
15	H^-	99	$C + e^- \rightarrow C^- + \gamma$	$k_{142} = 2.25 \times 10^{-15}$		81
16	He^-	100	$C + H \rightarrow CH + \gamma$	$k_{143} = 1.0 \times 10^{-17}$		82
	$OH + H \rightarrow$	101	$C + H_2 \rightarrow CH_2 + \gamma$	$k_{144} = 1.0 \times 10^{-17}$		82
	$OH + H_2 \rightarrow$	102	$C + C \rightarrow C_2 + \gamma$	$k_{145} = 4.36 \times 10^{-18} \left(\frac{T}{300}\right)^{0.35} \exp\left(-\frac{161.3}{T}\right)$		83
	$OH + C \rightarrow$	103	$C + O \rightarrow CO + \gamma$	$k_{146} = 2.1 \times 10^{-19}$		84
	$OH + O \rightarrow$	104		$= 3.09 \times 10^{-17} \left(\frac{T}{300}\right)^{0.33} \exp\left(-\frac{1629}{T}\right)$		85
	$OH + OH \rightarrow$	105	$C^+ + H \rightarrow CH^+ + \gamma$	$k_{147} = 4.46 \times 10^{-16} T^{-0.5} \exp\left(-\frac{4.93}{T^{2/3}}\right)$		86
	$H_2O + H \rightarrow$	106	$C^+ + H_2 \rightarrow CH_2^+ + \gamma$	$k_{148} = 4.0 \times 10^{-16} \left(\frac{T}{300}\right)^{-0.2}$		87
17	He^+	107	$C^+ + O \rightarrow CO^+ + \gamma$	$k_{149} = 2.5 \times 10^{-18}$		84
	$O_2 + H \rightarrow$	108		$= 3.14 \times 10^{-18} \left(\frac{T}{300}\right)^{-0.15} \exp\left(\frac{68}{T}\right)$		84
	$O_2 + H_2 \rightarrow$	109	$O + e^- \rightarrow O^- + \gamma$	$k_{150} = 1.5 \times 10^{-15}$		28
	$O_2 + C \rightarrow$	110	$O + H \rightarrow OH + \gamma$	$k_{151} = 9.9 \times 10^{-19} \left(\frac{T}{300}\right)^{-0.38}$		28
	$CO + H \rightarrow$	111	$O + O \rightarrow O_2 + \gamma$	$k_{152} = 4.9 \times 10^{-20} \left(\frac{T}{300}\right)^{1.58}$		82
	$H_2^+ + H_2 \rightarrow$	112	$OH + H \rightarrow H_2O + \gamma$	$k_{153} = 5.26 \times 10^{-18} \left(\frac{T}{300}\right)^{-5.22} \exp\left(-\frac{90}{T}\right)$		88
18	He^+	113	$H + H + H \rightarrow H_2 + H$	$k_{154} = 1.32 \times 10^{-32} \left(\frac{T}{300}\right)^{-0.38}$		89
19	He^+	114		$= 1.32 \times 10^{-32} \left(\frac{T}{300}\right)^{-1.0}$		90
	$C + H_2^+ \rightarrow$	115	$H + H + H_2 \rightarrow H_2 + H_2$	$k_{155} = 2.8 \times 10^{-31} T^{-0.6}$		91
20	C^+	116	$H + H + He \rightarrow H_2 + He$	$k_{156} = 6.9 \times 10^{-32} T^{-0.4}$		92
	$C + H_3^+ \rightarrow$	117	$C + C + M \rightarrow C_2 + M$	$k_{157} = 5.99 \times 10^{-33} \left(\frac{T}{5000}\right)^{-1.6}$		93
	$C^+ + H_2 \rightarrow$	118		$= 5.99 \times 10^{-33} \left(\frac{T}{5000}\right)^{-0.64} \exp\left(\frac{5455}{T}\right)$		94
	$CH^+ + H \rightarrow$	119	$C + O + M \rightarrow CO + M$	$k_{158} = 6.16 \times 10^{-29} \left(\frac{T}{300}\right)^{-3.08}$		35
	$CH^+ + H_2 \rightarrow$	120		$= 2.14 \times 10^{-29} \left(\frac{T}{300}\right)^{-3.08} \exp\left(\frac{2114}{T}\right)$		67
	$CH_2^+ + H \rightarrow$	121	$C^+ + O + M \rightarrow CO^+ + M$	$k_{159} = 100 \times k_{210}$		67
	$O + H_2 \rightarrow$	122	$C + O^+ + M \rightarrow CO^+ + M$	$k_{160} = 100 \times k_{210}$		67
	$O + H \rightarrow$	123	$O + H + M \rightarrow OH + M$	$k_{161} = 4.33 \times 10^{-32} \left(\frac{T}{300}\right)^{-1.0}$		43
	$O + H_3^+ \rightarrow$	124	$OH + H + M \rightarrow H_2O + M$	$k_{162} = 2.56 \times 10^{-31} \left(\frac{T}{300}\right)^{-2.0}$		35
	$O + H_2 \rightarrow$	125	$O + O + M \rightarrow O_2 + M$	$k_{163} = 9.2 \times 10^{-34} \left(\frac{T}{300}\right)^{-1.0}$		37
	$O + H_2^+ \rightarrow$	126	$O + CH \rightarrow HCO^+ + e^-$	$k_{164} = 2.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.44}$		95
27	C^+	127	$H + H(s) \rightarrow H_2$	$k_{165} = 3.0 \times 10^{-18} T^{0.5} f_A [1.0 + 0.04(T + T_d)^{0.5}]$		96
28	C^+	128		$f_A = [1.0 + 10^4 \exp\left(-\frac{600}{T_d}\right)]^{-1}$		
29	C^+	129		$+ 0.002 T + 8 \times 10^{-6} T^2]$		
	$OH^+ + H_2 \rightarrow$	130	$HCO^+ + e^- \rightarrow CO + H$	$k_{129} = 2.76 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.64}$	79	
	$H_2O^+ + H \rightarrow$	131	$HCO^+ + e^- \rightarrow OH + C$	$k_{130} = 2.4 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.64}$	79	
	$H_2O + H_3^+ \rightarrow$	132	$HOC^+ + e^- \rightarrow CO + H$	$k_{131} = 1.1 \times 10^{-7} \left(\frac{T}{300}\right)^{-1.0}$	28	
	$H_2O + C^+ \rightarrow$	133	$H^- + C \rightarrow CH + e^-$	$k_{132} = 1.0 \times 10^{-9}$	28	
	$H_2O + C^+ \rightarrow$	134	$H^- + O \rightarrow OH + e^-$	$k_{133} = 1.0 \times 10^{-9}$	28	
	$H_3O^+ + C \rightarrow$	135	$H^- + OH \rightarrow H_2O + e^-$	$k_{134} = 1.0 \times 10^{-10}$	28	
31	OH	136	$C^- + H \rightarrow CH + e^-$	$k_{135} = 5.0 \times 10^{-10}$	28	
	$O_2 + C^+ \rightarrow$	137	$C^- + H_2 \rightarrow CH_2 + e^-$	$k_{136} = 1.0 \times 10^{-13}$	28	
	$O_2 + C^+ \rightarrow$	138	$C^- + O \rightarrow CO + e^-$	$k_{137} = 5.0 \times 10^{-10}$	28	
	$CO + H_3^+ \rightarrow$	139	$O^- + H \rightarrow OH + e^-$	$k_{138} = 5.0 \times 10^{-10}$	28	
	$CO + H_3^+ \rightarrow$	140	$O^- + H_2 \rightarrow H_2O + e^-$	$k_{139} = 7.0 \times 10^{-10}$	28	
	$HCO^+ + C \rightarrow$	141	$O^- + C \rightarrow CO + e^-$	$k_{140} = 5.0 \times 10^{-10}$	28	
	$HCO^+ + H_2O \rightarrow$	142	$HCO^+ + H_2O \rightarrow CO + H_3O^+$	$k_{87} = 2.5 \times 10^{-3}$		



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14	$H^- + H \rightarrow H + H + e^-$	88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$	63
	36 $CH + H_2 \rightarrow$	89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$	63
	37 $CH + C \rightarrow$	90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$	28
	38 $CH_2 + O \rightarrow$	91	$CH_2 + H \rightarrow CH_2^+ + H$	$k_{91} = 1.4 \times 10^{-9}$	28
		92	$CH_2 + H^+ \rightarrow CH_2^+ + e^- + H_2$	$k_{92} = 5.5 \times 10^{-11}$	28
	39 $C_2 + O \rightarrow$	93	$C_2 + He^+ \rightarrow C^+ + C^+ + e^- + e^-$	$k_{93} = 6.5 \times 10^{-9}$	28
	40 $CH_2 + O \rightarrow$	94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-9}$	28
	41 $CH_2 + O \rightarrow$	95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$	28
	42 $C_2 + O \rightarrow$	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	$H_2O + H^+ \rightarrow OH^+ + H + H^+$	$k_{98} = 0.86 \times 10^{-10}$	65

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

No.	Reaction	Optically thin rate (s^{-1})	γ	Ref.				
166	$\text{H}^- + \gamma \rightarrow \text{H} + \text{e}^-$	$R_{166} = 7.1 \times 10^{-7}$	0.5	1	$36 \times 10^{-18} \left(\frac{T}{300}\right)^{0.35} \exp\left(-\frac{161.3}{T}\right)$			82
167	$\text{H}_2^+ + \gamma \rightarrow \text{H} + \text{H}^+$	$R_{167} = 1.1 \times 10^{-9}$	1.9	2	1×10^{-19}	$T \leq 300 \text{ K}$		83
168	$\text{H}_2 + \gamma \rightarrow \text{H} + \text{H}$	$R_{168} = 5.6 \times 10^{-11}$	See §2.2	3	$0.9 \times 10^{-17} \left(\frac{T}{300}\right)^{0.33} \exp\left(-\frac{1629}{T}\right)$	$T > 300 \text{ K}$		84
169	$\text{H}_3^+ + \gamma \rightarrow \text{H}_2 + \text{H}^+$	$R_{169} = 4.9 \times 10^{-13}$	1.8	4	$46 \times 10^{-16} T^{-0.5} \exp\left(-\frac{4.93}{T^{2/3}}\right)$			85
170	$\text{H}_3^+ + \gamma \rightarrow \text{H}_2^+ + \text{H}$	$R_{170} = 4.9 \times 10^{-13}$	2.3	4	$0 \times 10^{-16} \left(\frac{T}{300}\right)^{-0.2}$			86
171	$\text{C} + \gamma \rightarrow \text{C}^+ + \text{e}^-$	$R_{171} = 3.1 \times 10^{-10}$	3.0	5	$5 \times 10^{-18} \left(\frac{T}{300}\right)^{-0.15} \exp\left(\frac{68}{T}\right)$	$T \leq 300 \text{ K}$		87
172	$\text{C}^- + \gamma \rightarrow \text{C} + \text{e}^-$	$R_{172} = 2.4 \times 10^{-7}$	0.9	6	5×10^{-15}	$T > 300 \text{ K}$		88
173	$\text{CH} + \gamma \rightarrow \text{C} + \text{H}$	$R_{173} = 8.7 \times 10^{-10}$	1.2	7	$9 \times 10^{-19} \left(\frac{T}{300}\right)^{-0.38}$			89
174	$\text{CH} + \gamma \rightarrow \text{CH}^+ + \text{e}^-$	$R_{174} = 7.7 \times 10^{-10}$	2.8	8	$9 \times 10^{-20} \left(\frac{T}{300}\right)^{1.58}$			90
175	$\text{CH}^+ + \gamma \rightarrow \text{C} + \text{H}^+$	$R_{175} = 2.6 \times 10^{-10}$	2.5	7	$26 \times 10^{-18} \left(\frac{T}{300}\right)^{-5.22} \exp\left(-\frac{90}{T}\right)$			91
176	$\text{CH}_2 + \gamma \rightarrow \text{CH} + \text{H}$	$R_{176} = 7.1 \times 10^{-10}$	1.7	7	$32 \times 10^{-32} \left(\frac{T}{300}\right)^{-0.38}$	$T \leq 300 \text{ K}$		92
177	$\text{CH}_2 + \gamma \rightarrow \text{CH}_2^+ + \text{e}^-$	$R_{177} = 5.9 \times 10^{-10}$	2.3	6	$32 \times 10^{-32} \left(\frac{T}{300}\right)^{-1.0}$	$T > 300 \text{ K}$		93
178	$\text{CH}_2^+ + \gamma \rightarrow \text{CH}^+ + \text{H}$	$R_{178} = 4.6 \times 10^{-10}$	1.7	9	$8 \times 10^{-31} T^{-0.6}$			94
179	$\text{CH}_3^+ + \gamma \rightarrow \text{CH}_2^+ + \text{H}$	$R_{179} = 1.0 \times 10^{-9}$	1.7	6	$9 \times 10^{-32} T^{-0.4}$			95
180	$\text{CH}_3^+ + \gamma \rightarrow \text{CH}^+ + \text{H}_2$	$R_{180} = 1.0 \times 10^{-9}$	1.7	6	$99 \times 10^{-33} \left(\frac{T}{5000}\right)^{-1.6}$	$T \leq 5000 \text{ K}$		96
181	$\text{C}_2 + \gamma \rightarrow \text{C} + \text{C}$	$R_{181} = 1.5 \times 10^{-10}$	2.1	7	$99 \times 10^{-33} \left(\frac{T}{5000}\right)^{-0.64} \exp\left(\frac{5255}{T}\right)$	$T > 5000 \text{ K}$		97
182	$\text{O}^- + \gamma \rightarrow \text{O} + \text{e}^-$	$R_{182} = 2.4 \times 10^{-7}$	0.5	6	$16 \times 10^{-29} \left(\frac{T}{300}\right)^{-3.08}$	$T \leq 2000 \text{ K}$		98
183	$\text{OH} + \gamma \rightarrow \text{O} + \text{H}$	$R_{183} = 3.7 \times 10^{-10}$	1.7	10	$14 \times 10^{-29} \left(\frac{T}{300}\right)^{-3.08} \exp\left(\frac{2114}{T}\right)$	$T > 2000 \text{ K}$		99
184	$\text{OH} + \gamma \rightarrow \text{OH}^+ + \text{e}^-$	$R_{184} = 1.6 \times 10^{-12}$	3.1	6	$10 \times k_{210}$			100
185	$\text{OH}^+ + \gamma \rightarrow \text{O} + \text{H}^+$	$R_{185} = 1.0 \times 10^{-12}$	1.8	4	$10 \times k_{210}$			101
186	$\text{H}_2\text{O} + \gamma \rightarrow \text{OH} + \text{H}$	$R_{186} = 6.0 \times 10^{-10}$	1.7	11	$33 \times 10^{-32} \left(\frac{T}{300}\right)^{-1.0}$			102
187	$\text{H}_2\text{O} + \gamma \rightarrow \text{H}_2\text{O}^+ + \text{e}^-$	$R_{187} = 3.2 \times 10^{-11}$	3.9	8	$56 \times 10^{-31} \left(\frac{T}{300}\right)^{-2.0}$			103
188	$\text{H}_2\text{O}^+ + \gamma \rightarrow \text{H}_2^+ + \text{O}$	$R_{188} = 5.0 \times 10^{-11}$	See §2.2	12	$2 \times 10^{-34} \left(\frac{T}{300}\right)^{-1.0}$			104
189	$\text{H}_2\text{O}^+ + \gamma \rightarrow \text{H}^+ + \text{OH}$	$R_{189} = 5.0 \times 10^{-11}$	See §2.2	12	$0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.44}$			105
190	$\text{H}_2\text{O}^+ + \gamma \rightarrow \text{O}^+ + \text{H}_2$	$R_{190} = 5.0 \times 10^{-11}$	See §2.2	12	$0 \times 10^{-18} T^{0.5} f_{\text{A}} [1.0 + 0.04(T + T_d)^{0.5}]$	$f_{\text{A}} = [1.0 + 10^4 \exp\left(-\frac{600}{T_d}\right)]^{-1}$		106
191	$\text{H}_2\text{O}^+ + \gamma \rightarrow \text{OH}^+ + \text{H}$	$R_{191} = 1.5 \times 10^{-10}$	See §2.2	12	$0.002 T + 8 \times 10^{-6} T^2]^{-1}$			107
192	$\text{H}_3\text{O}^+ + \gamma \rightarrow \text{H}^+ + \text{H}_2\text{O}$	$R_{192} = 2.5 \times 10^{-11}$	See §2.2	12	$6 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.64}$		79	108
193	$\text{H}_3\text{O}^+ + \gamma \rightarrow \text{H}_2^+ + \text{OH}$	$R_{193} = 2.5 \times 10^{-11}$	See §2.2	12	$\times 10^{-8} \left(\frac{T}{300}\right)^{-0.64}$		79	109
194	$\text{H}_3\text{O}^+ + \gamma \rightarrow \text{H}_2\text{O}^+ + \text{H}$	$R_{194} = 7.5 \times 10^{-12}$	See §2.2	12	$\times 10^{-7} \left(\frac{T}{300}\right)^{-1.0}$		28	110
195	$\text{H}_3\text{O}^+ + \gamma \rightarrow \text{OH}^+ + \text{H}_2$	$R_{195} = 2.5 \times 10^{-11}$	See §2.2	12	$\times 10^{-9}$		28	111
196	$\text{O}_2 + \gamma \rightarrow \text{O}_2^+ + \text{e}^-$	$R_{196} = 5.6 \times 10^{-11}$	3.7	7	$\times 10^{-9}$		28	112
197	$\text{O}_2 + \gamma \rightarrow \text{O} + \text{O}$	$R_{197} = 7.0 \times 10^{-10}$	1.8	7	$\times 10^{-10}$		28	113
198	$\text{CO} + \gamma \rightarrow \text{C} + \text{O}$	$R_{198} = 2.0 \times 10^{-10}$	See §2.2	13	$\times 10^{-10}$		28	114



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14	$H^- + H \rightarrow H + H + e^-$	88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$	63
36	$CH + H_2^- \rightarrow$	89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$	63
37	$CH + C^- \rightarrow$	90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$	28
38	$CH + C^- \rightarrow$	91	$CH_2 + H^+ \rightarrow CH_2^+ + H$	$k_{91} = 1.4 \times 10^{-9}$	28
	$CH_2 + H^+ \rightarrow C^+ + e^- + H_2$			1.2×10^{-11}	28
39	$C_2 + H^- \rightarrow$	93	$C_2 + H^+ \rightarrow C^+ + C^+ + e^-$	$k_{93} = 6.1 \times 10^{-9}$	28
40	$CH_2 + O^- \rightarrow$	94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-9}$	28
41	$CH_2 + O^- \rightarrow$	95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$	28
	$CH_2 + O^- \rightarrow$	96	$H_2O + H^+ \rightarrow H_2O^+ + H$	$k_{96} = 6.9 \times 10^{-9}$	64
42	$C_2 + O \rightarrow$	97	$H_2O + He^+ \rightarrow OH + He + H^+$	$k_{97} = 2.04 \times 10^{-10}$	65
	$C_2 + O \rightarrow$	98	$CO + H^+ \rightarrow CO^+ + H$	$\approx 2.04 \times 10^{-10}$	65

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

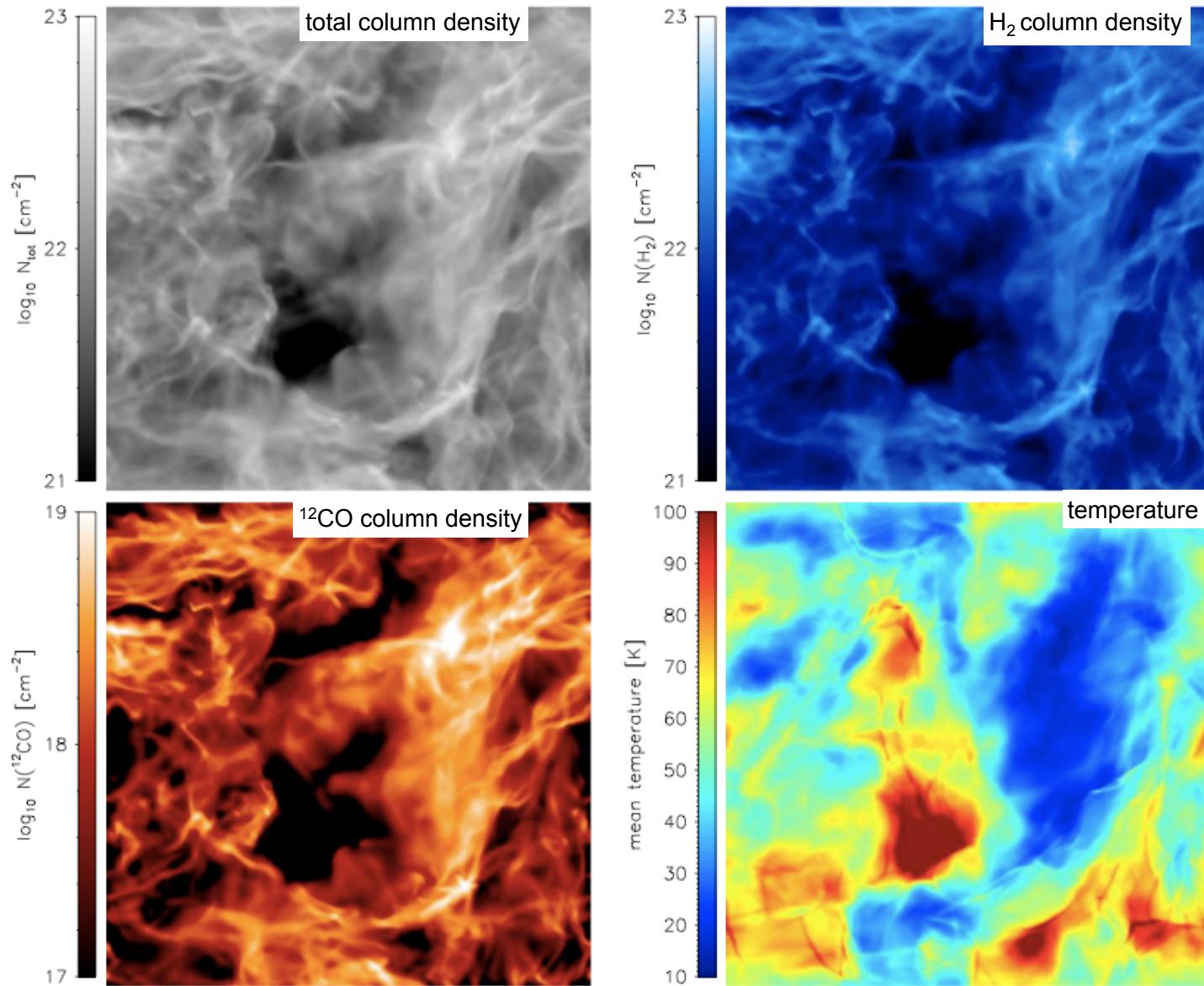
No.	Reaction	Optically thin rate (s^{-1})	γ	Ref.
166	$H^- + \gamma \rightarrow H + e^-$	$R_{166} = 7.1 \times 10^{-7}$	0.5	1
167	$H_2^+ + \gamma \rightarrow H + H^+$	$R_{167} = 1.1 \times 10^{-9}$	1.9	2
168	$H_2 + \gamma \rightarrow H + H$	$R_{168} = 5.6 \times 10^{-11}$	See §2.2	3
169	$H_3^+ + \gamma \rightarrow H_2 + H^+$	$R_{169} = 4.9 \times 10^{-13}$	1.8	4
170	$H_3^+ + \gamma \rightarrow H_2^+ + H$	$R_{170} = 4.9 \times 10^{-13}$	2.3	4
171	$C + \gamma \rightarrow C^+ + e^-$	$\approx 1 \times 10^{-10}$	$\approx \alpha$	$\approx \alpha$

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.
176	$CH_2 + \gamma$	199 $H + c.r. \rightarrow H^+ + e^-$	$R_{199} = 1.0$
177	$CH_2 + \gamma$	200 $He + c.r. \rightarrow He^+ + e^-$	$R_{200} = 1.1$
178	$CH_2^+ + \gamma$	201 $H_2 + c.r. \rightarrow H^+ + H + e^-$	$R_{201} = 0.037$
179	$CH_3^+ + \gamma$	202 $H_2 + c.r. \rightarrow H + H$	$R_{202} = 0.22$
180	$CH_3^+ + \gamma$	203 $H_2 + c.r. \rightarrow H^+ + H^-$	$R_{203} = 6.5 \times 10^{-4}$
181	$C_2 + \gamma \rightarrow$	204 $H_2 + c.r. \rightarrow H_2^+ + e^-$	$R_{204} = 2.0$
182	$O^- + \gamma \rightarrow$	205 $C + c.r. \rightarrow C^+ + e^-$	$R_{205} = 3.8$
183	$OH + \gamma \rightarrow$	206 $O + c.r. \rightarrow O^+ + e^-$	$R_{206} = 5.7$
184	$OH + \gamma \rightarrow$	207 $CO + c.r. \rightarrow CO^+ + e^-$	$R_{207} = 6.5$
185	$OH^+ + \gamma$	208 $C + \gamma_{c.r.} \rightarrow C^+ + e^-$	$R_{208} = 2800$
186	$H_2O + \gamma$	209 $CH + \gamma_{c.r.} \rightarrow C + H$	$R_{209} = 4000$
187	$H_2O + \gamma$	210 $CH^+ + \gamma_{c.r.} \rightarrow C^+ + H$	$R_{210} = 960$
188	$H_2O^+ + \gamma$	211 $CH_2 + \gamma_{c.r.} \rightarrow CH_2^+ + e^-$	$R_{211} = 2700$
189	$H_2O^+ + \gamma$	212 $CH_2 + \gamma_{c.r.} \rightarrow CH + H$	$R_{212} = 2700$
190	$H_2O^+ + \gamma$	213 $C_2 + \gamma_{c.r.} \rightarrow C + C$	$R_{213} = 1300$
191	$H_2O^+ + \gamma$	214 $OH + \gamma_{c.r.} \rightarrow O + H$	$R_{214} = 2800$
192	$H_3O^+ + \gamma$	215 $H_2O + \gamma_{c.r.} \rightarrow OH + H$	$R_{215} = 5300$
193	$H_3O^+ + \gamma$	216 $O_2 + \gamma_{c.r.} \rightarrow O + O$	$R_{216} = 4100$
194	$H_3O^+ + \gamma$	217 $O_2 + \gamma_{c.r.} \rightarrow O_2^+ + e^-$	$R_{217} = 640$
195	$H_3O^+ + \gamma$	218 $CO + \gamma_{c.r.} \rightarrow C + O$	$R_{218} = 0.21 T^{1/2} x_{H_2} x_{CO}^{-1/2}$
196	$O_2 + \gamma \rightarrow$		4
197	$O_2 + \gamma \rightarrow O + O$	$R_{197} = 7.0 \times 10^{-10}$	1.8
198	$CO + \gamma \rightarrow C + O$	$R_{198} = 2.0 \times 10^{-10}$	See §2.2

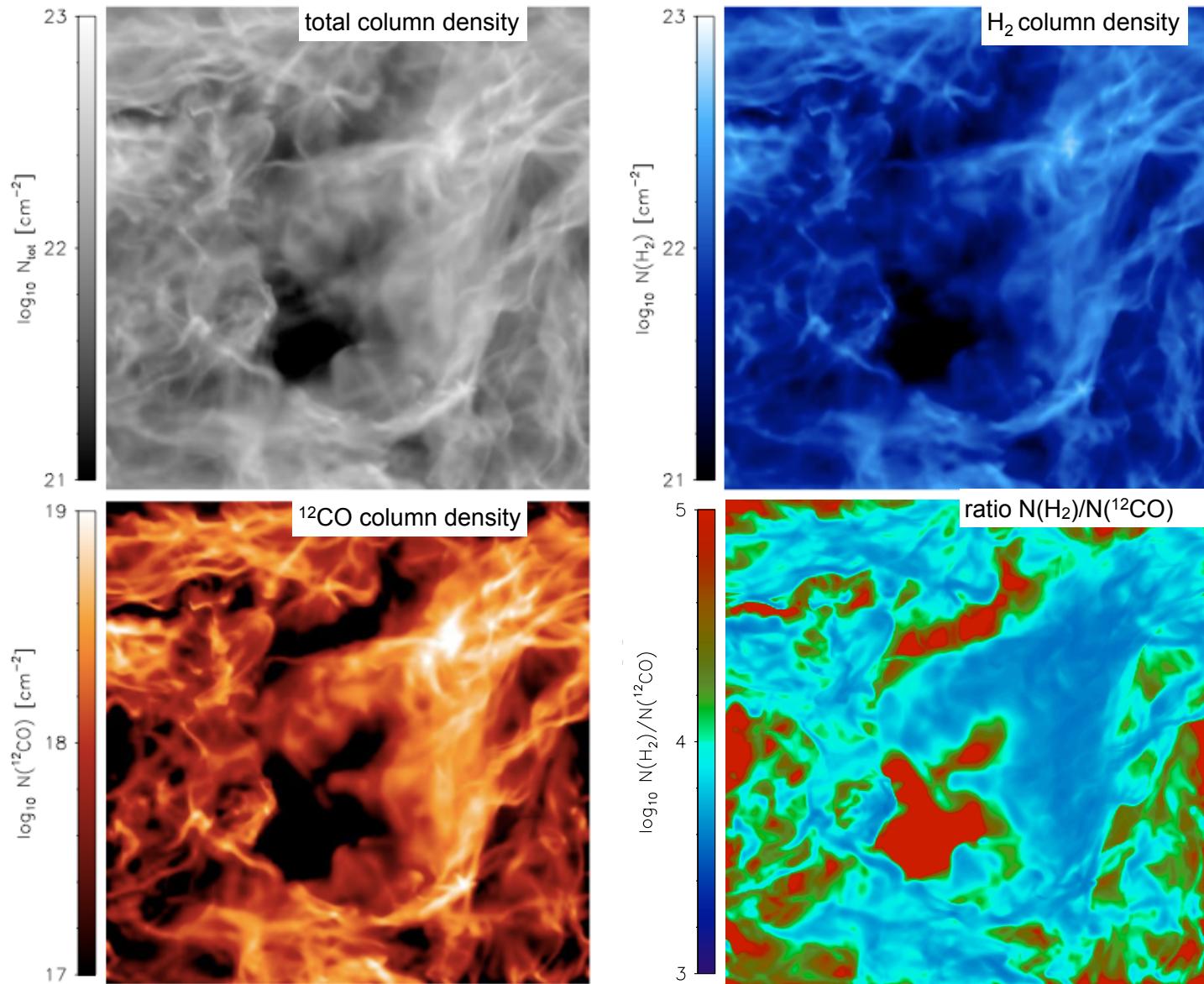
86	$HCO^+ + C \rightarrow$	140	$O^- + C \rightarrow CO + e^-$	$k_{140} = 5.0 \times 10^{-10}$
87	$HCO^+ + H_2O \rightarrow CO + H_3O^+$			$k_{87} = 2.5 \times 10^{-9}$

effects of chemistry



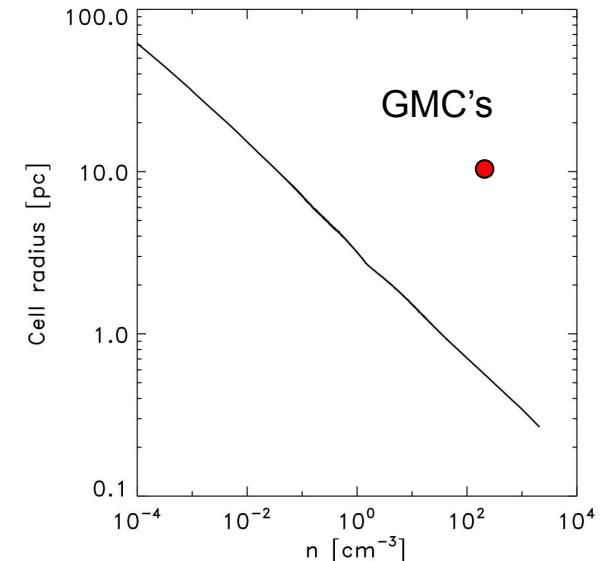
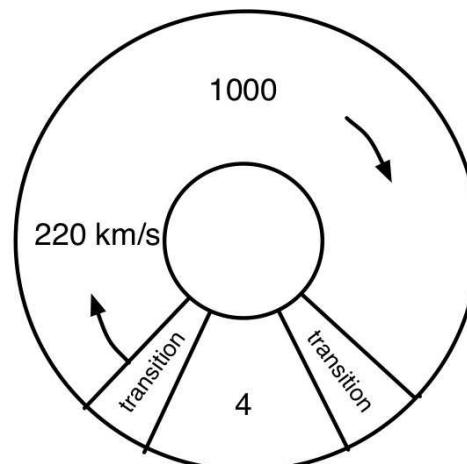
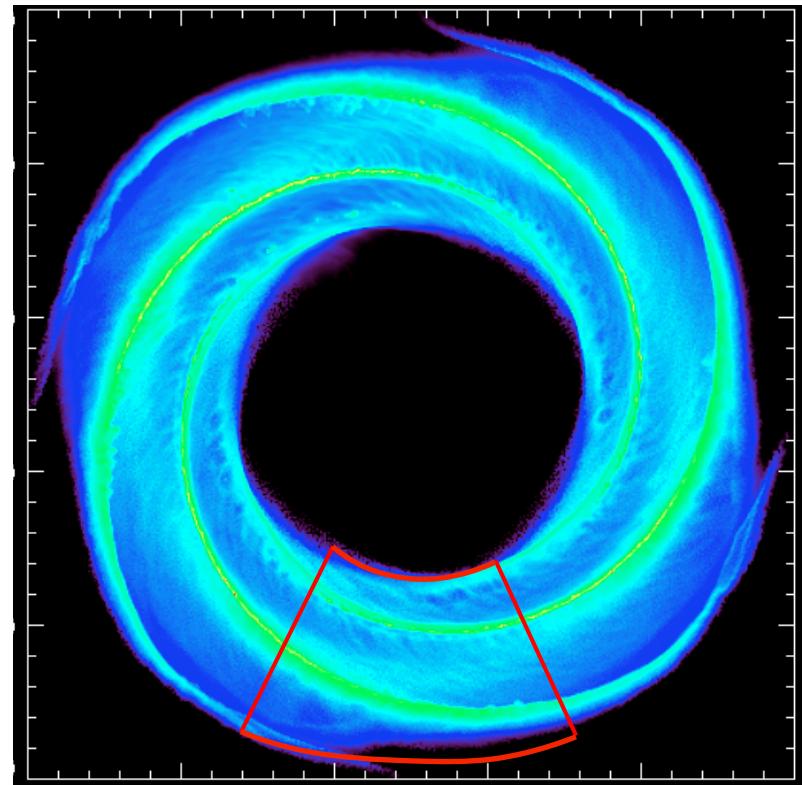
(Glover et al. 2010)

effects of chemistry



(Glover et al. 2010)

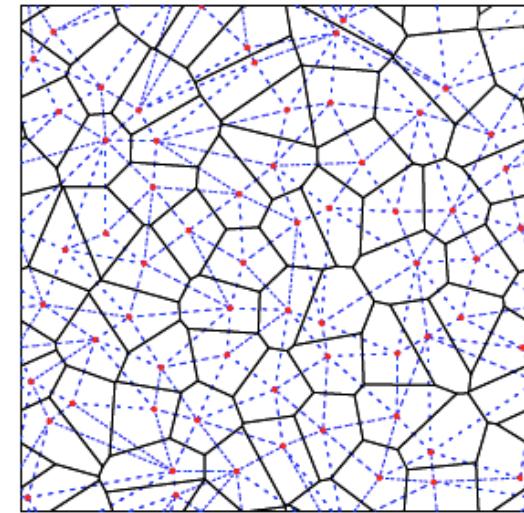
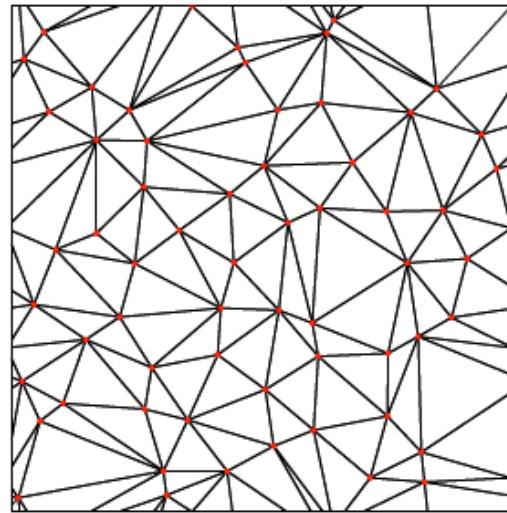
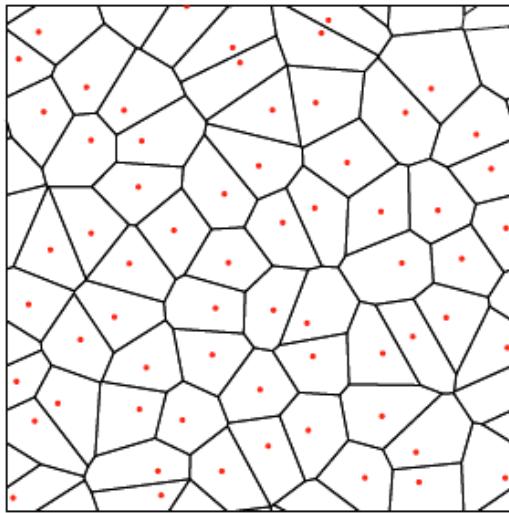
modeling molecular cloud formation



- 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

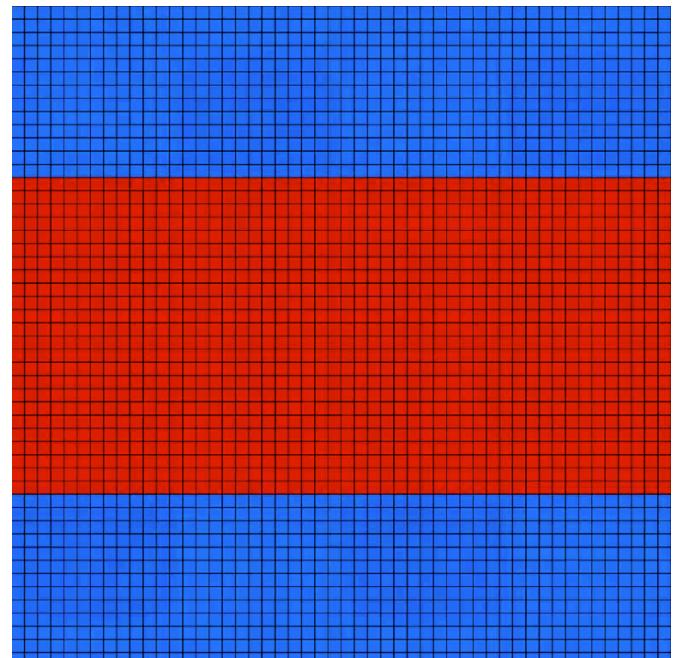
Simulation	Surface Density $M_{\odot} \text{ pc}^{-2}$	Radiation Field G_0
Milky Way	10	1
Low Density	4	1
Strong Field	10	10
Low & Weak	4	0.1

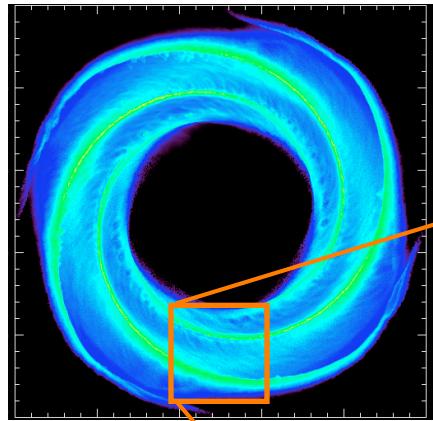
numerical method



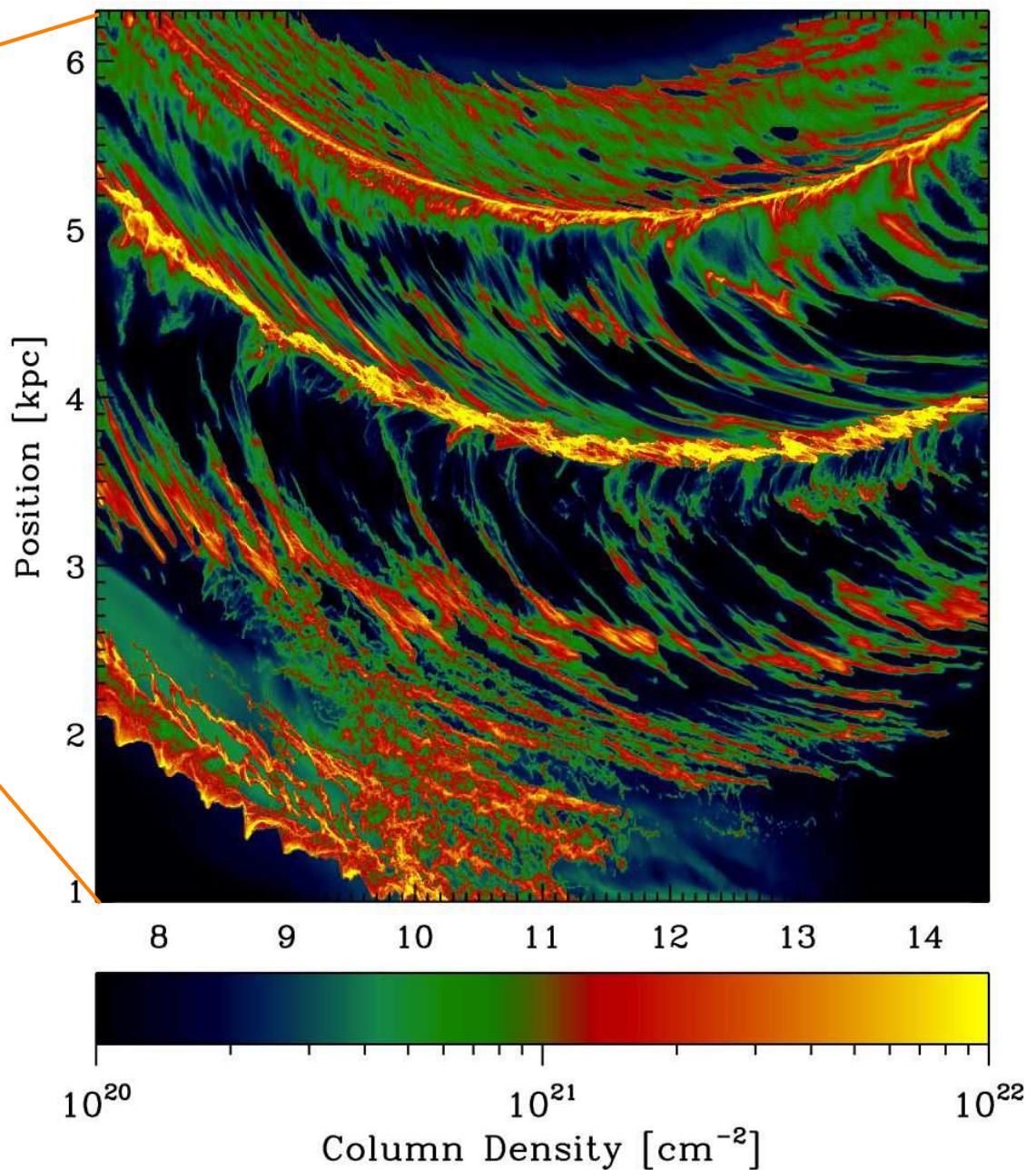
*moving mesh code **Arepo**:*

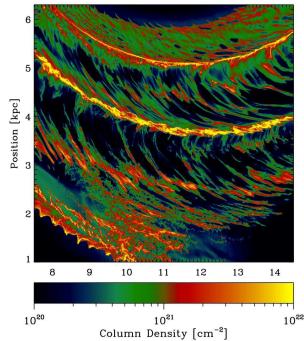
- semi-Lagrangian
- flexible refinement
- fluid instabilities and no artificial clumping
(Agertz et al. 2007)
- can also handle sub-sonic turbulence
(Bauer & Springel 2012)
- no preferred geometry



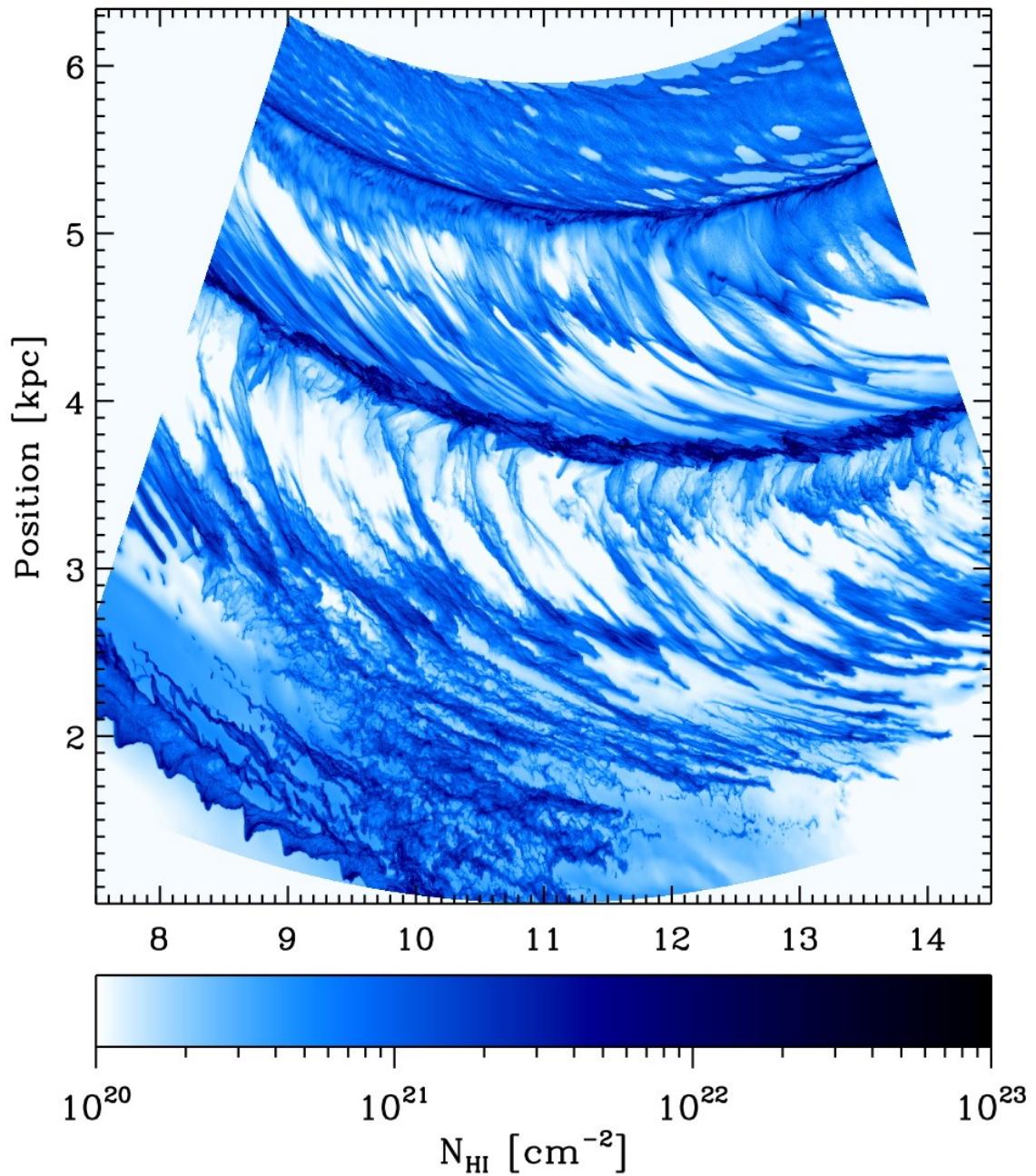


total column density

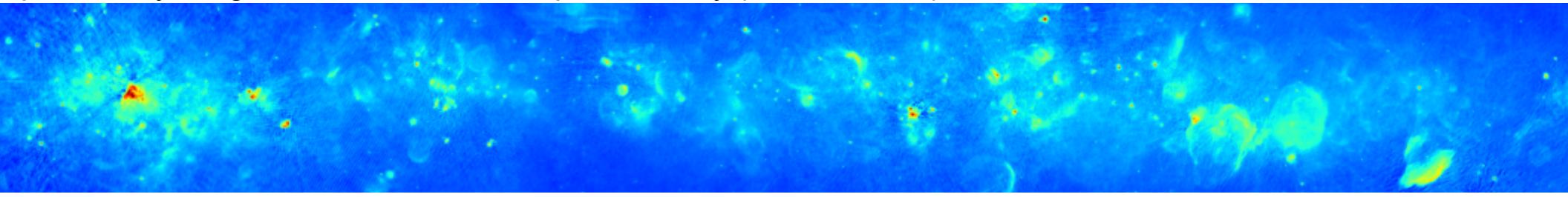




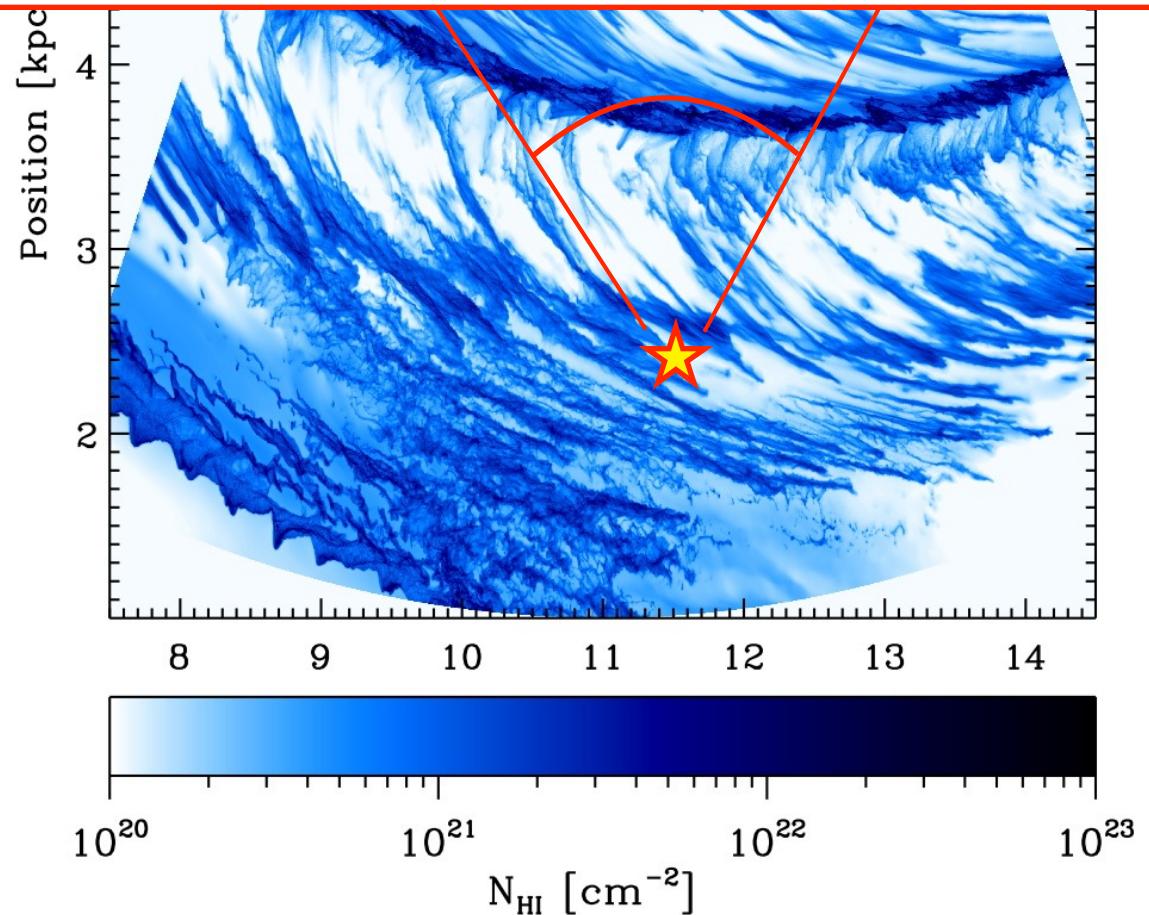
HI column density

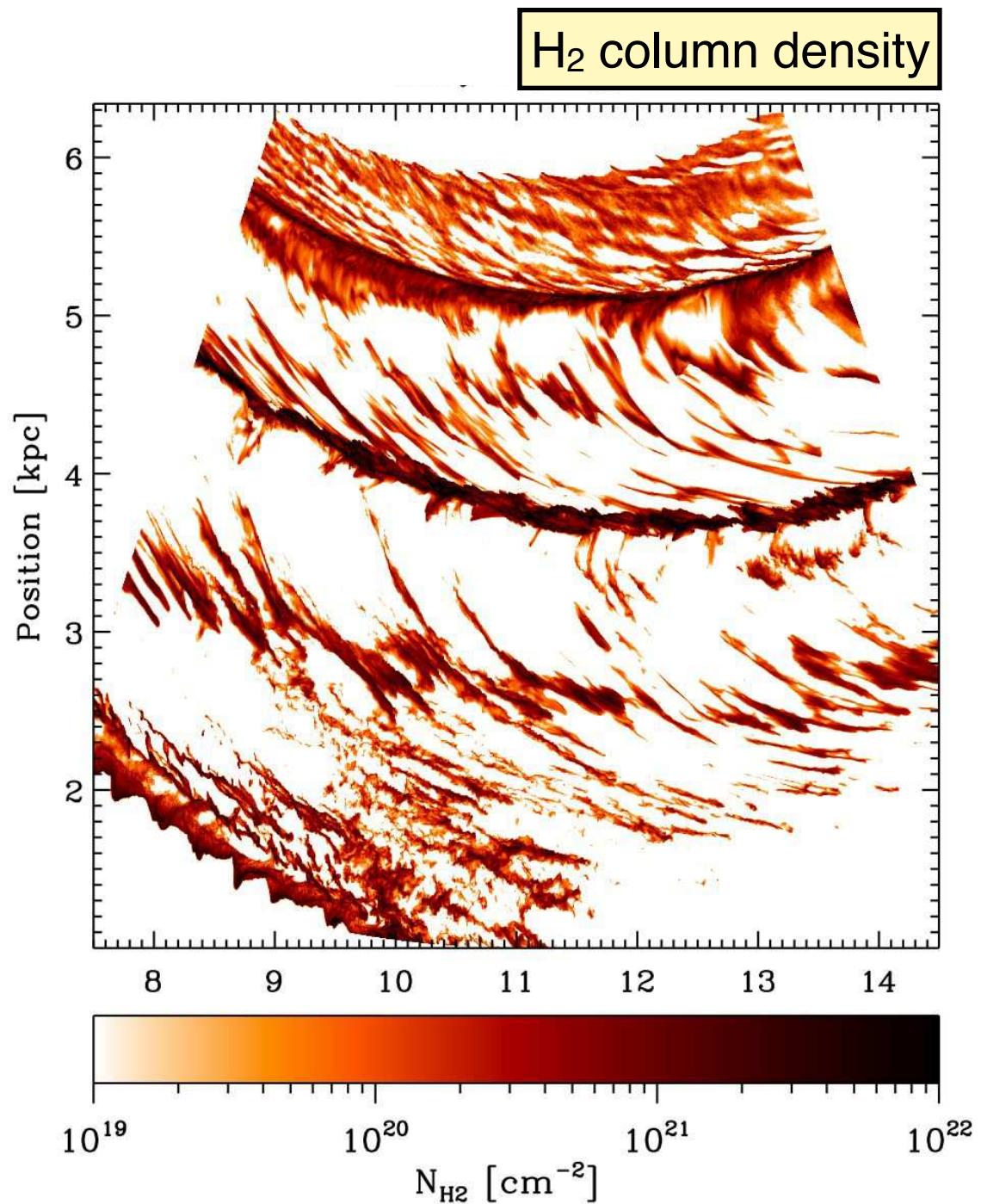
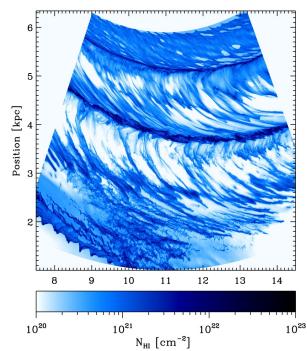
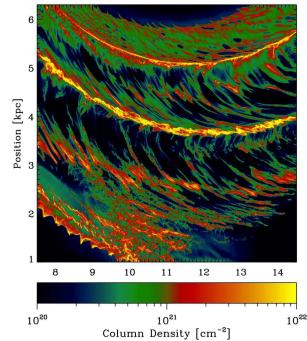


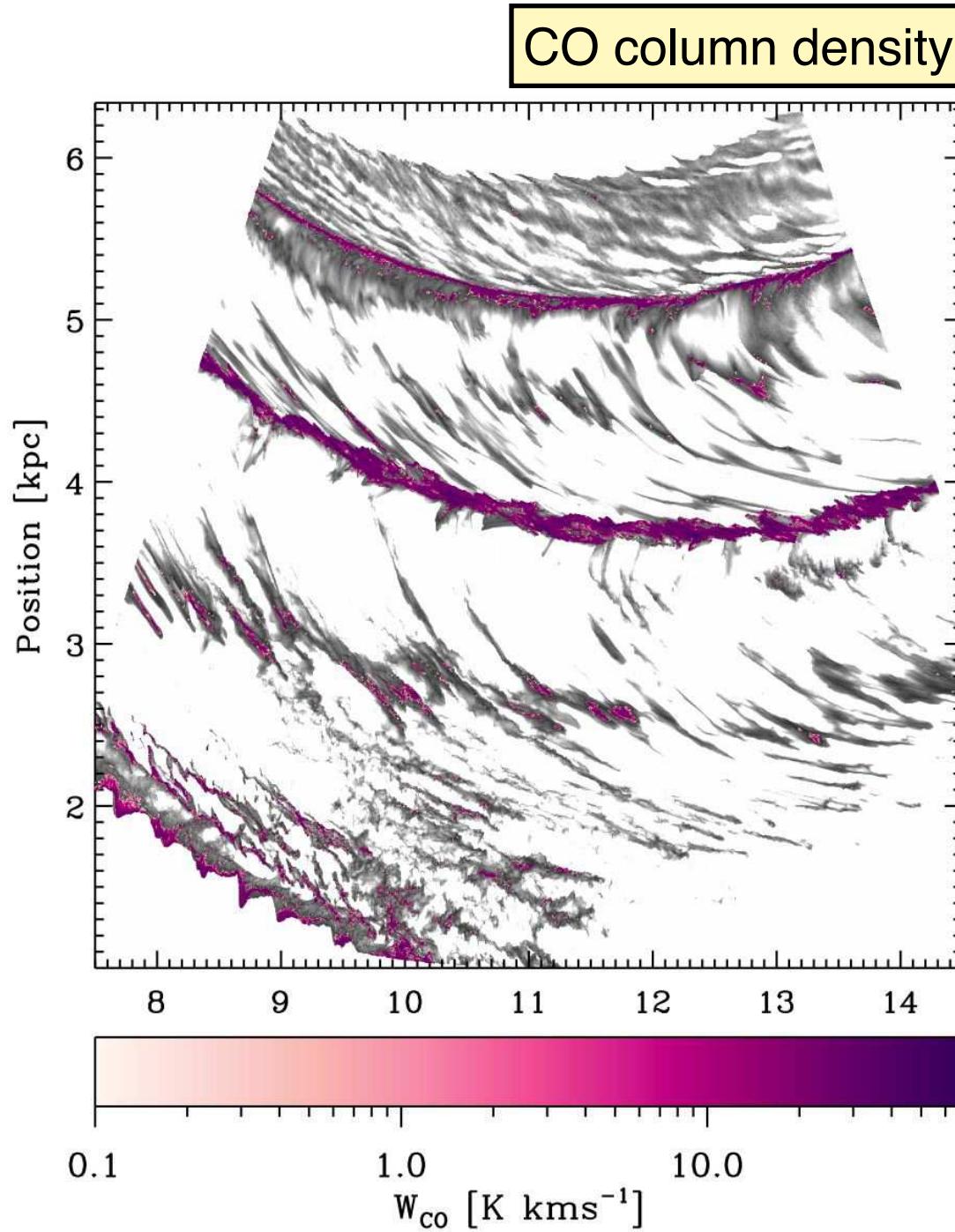
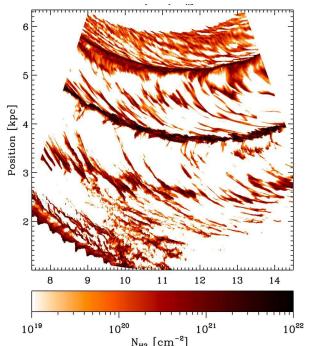
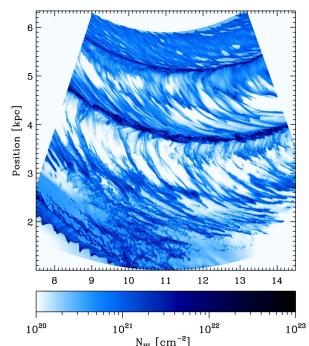
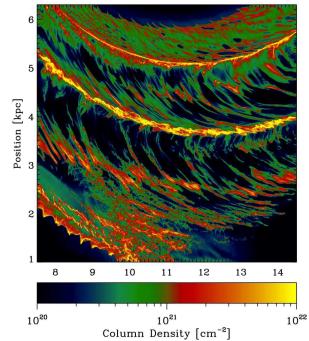
preliminary image from THOR Galactic plane survey (PI H. Beuther): continuum emission around 21 cm

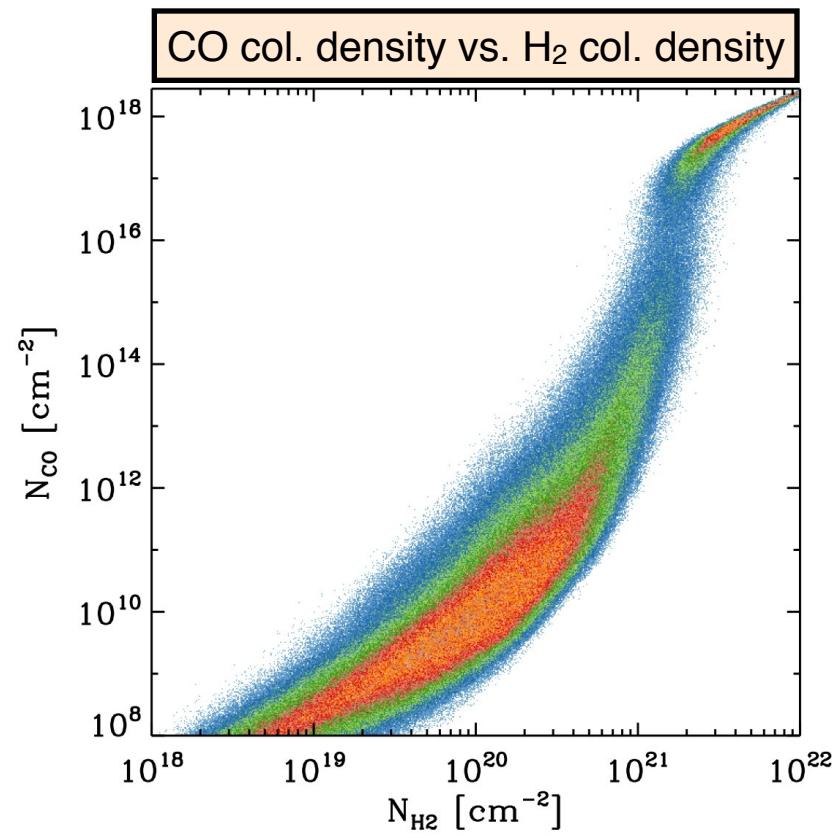
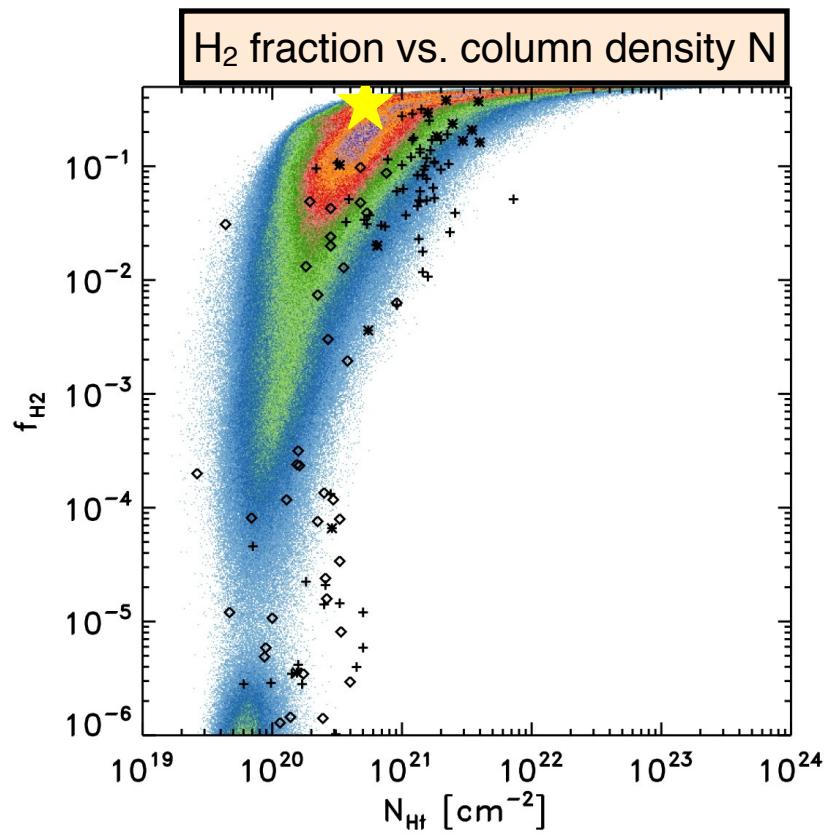


next step: produce all sky maps at various positions in the model galaxy (use RADMC-3D)





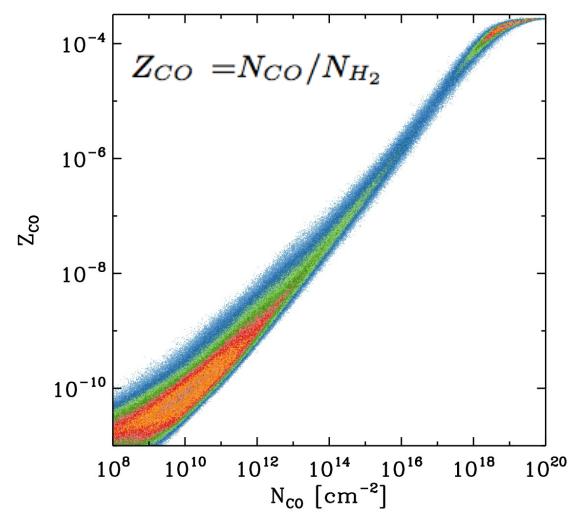




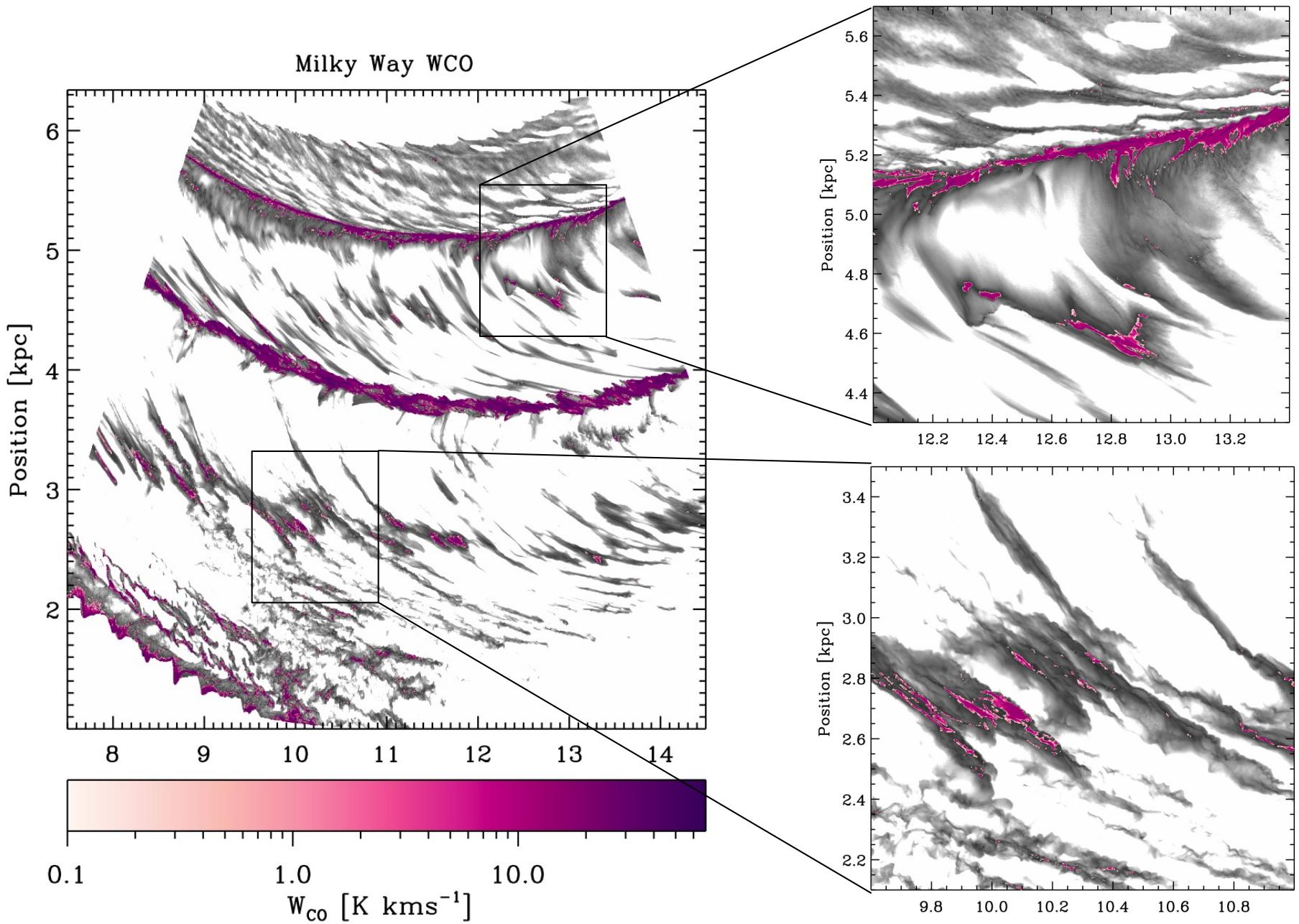
H₂ forms above column densities of 10^{20} cm^{-2}

CO columns jump after $N_{H_2} \sim 10^{21} \text{ cm}^{-2}$

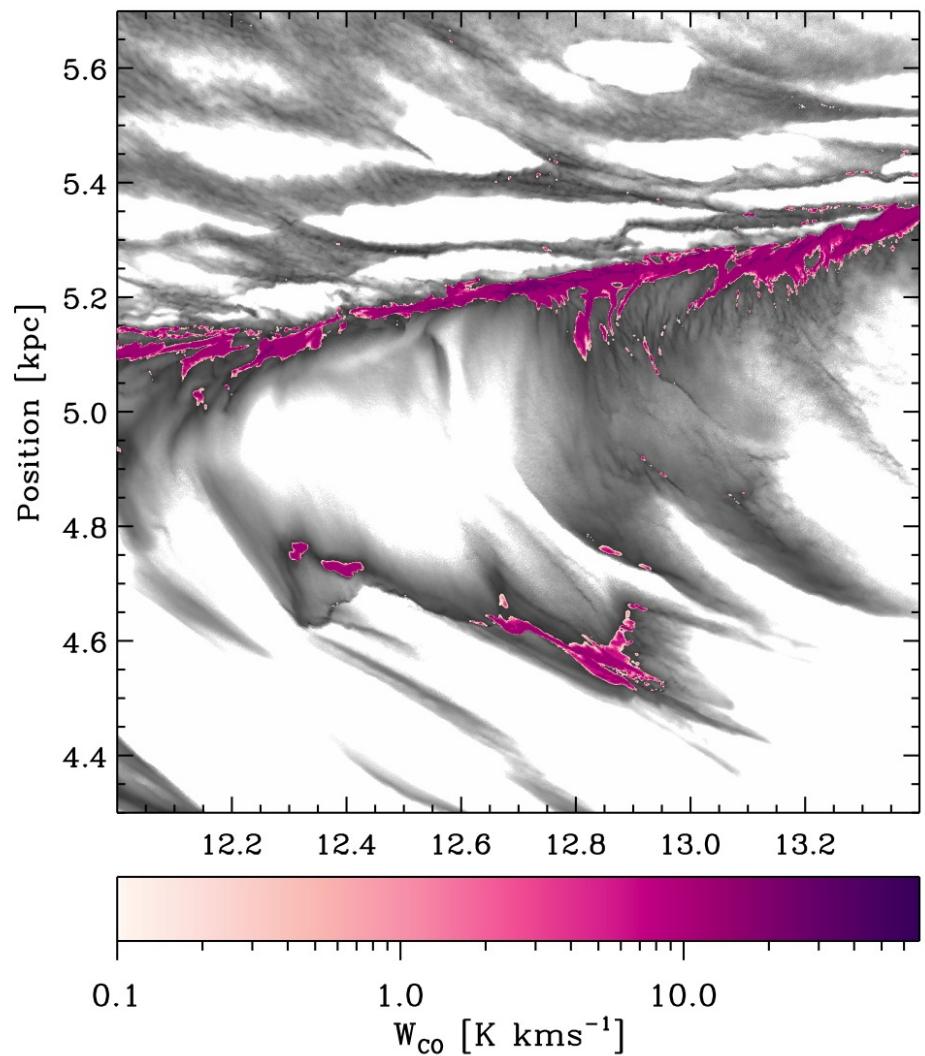
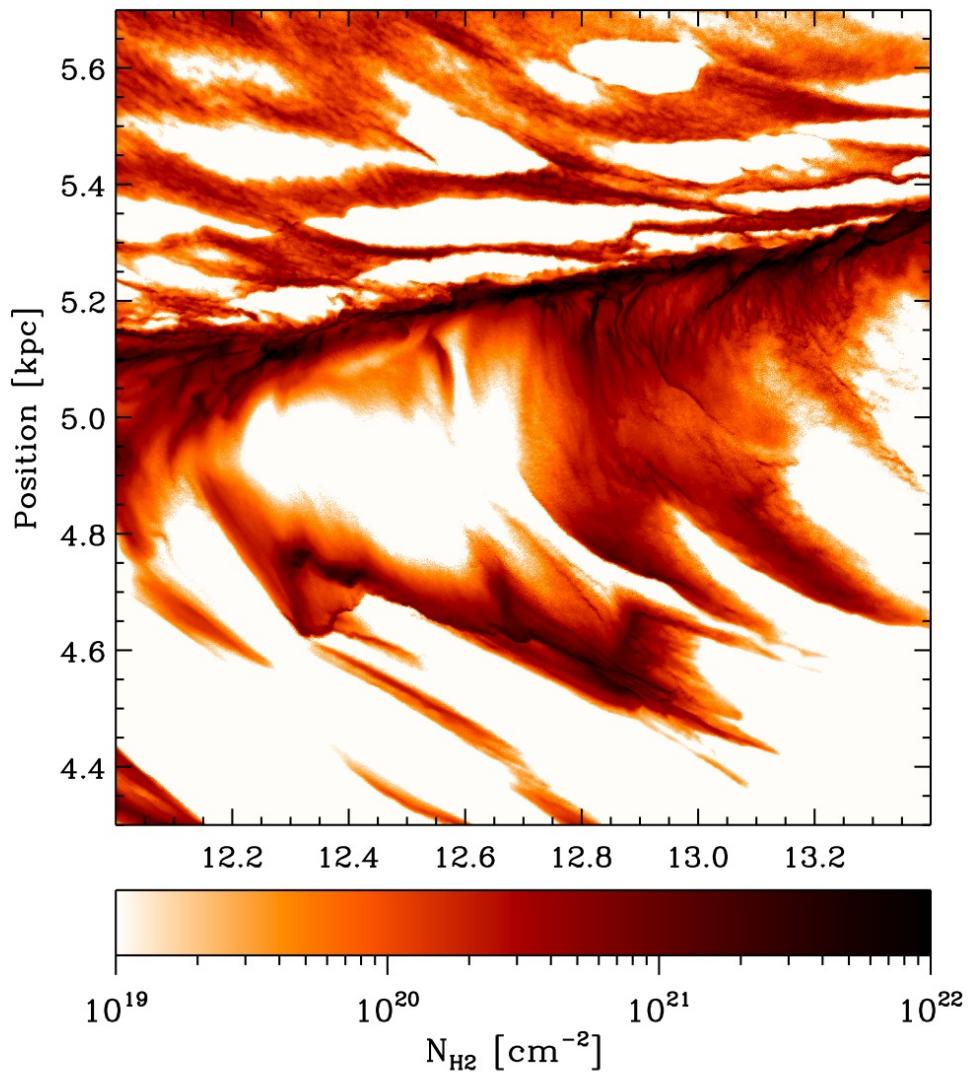
$$\log(Z_{CO}[\text{cm}^{-2}]) = -18.1 \log(N_{CO}[\text{cm}^{-2}]) + 0.8.$$



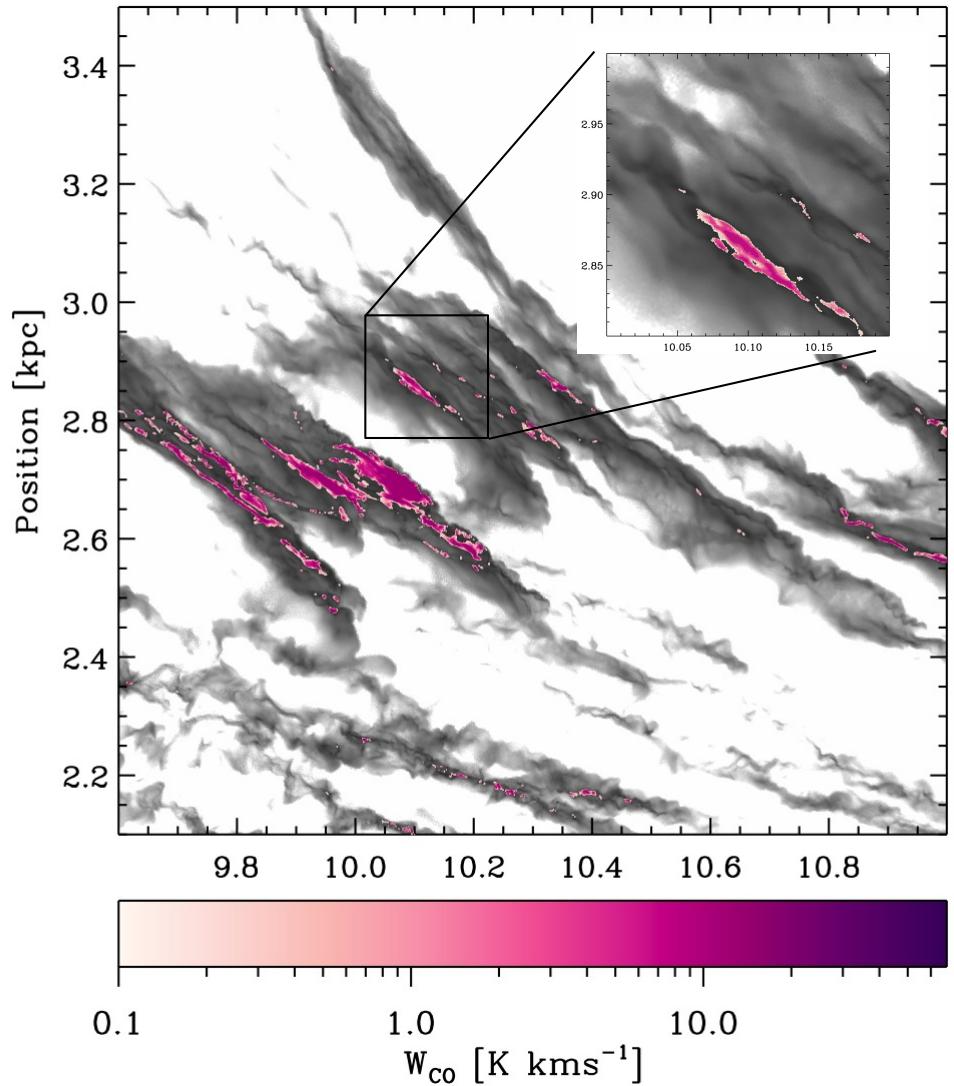
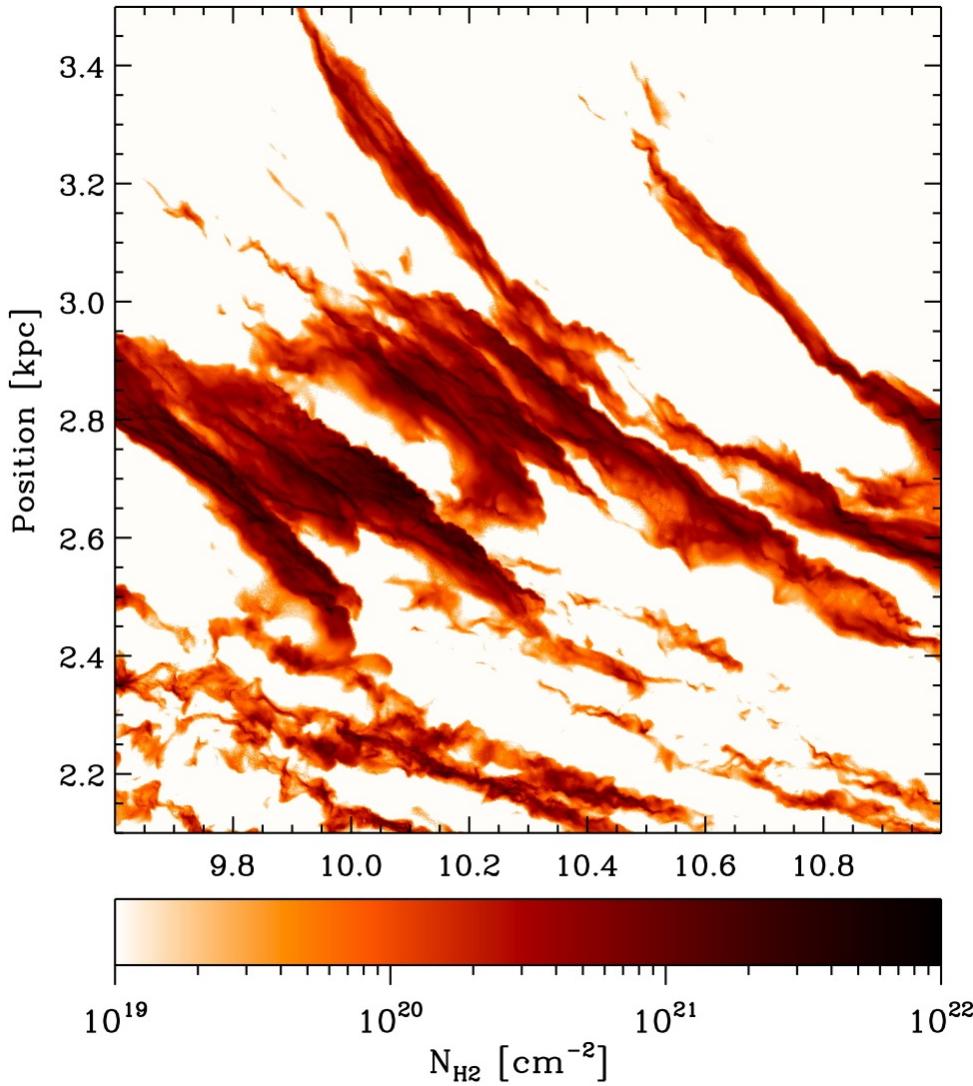
details of CO emission



relation between CO and H₂

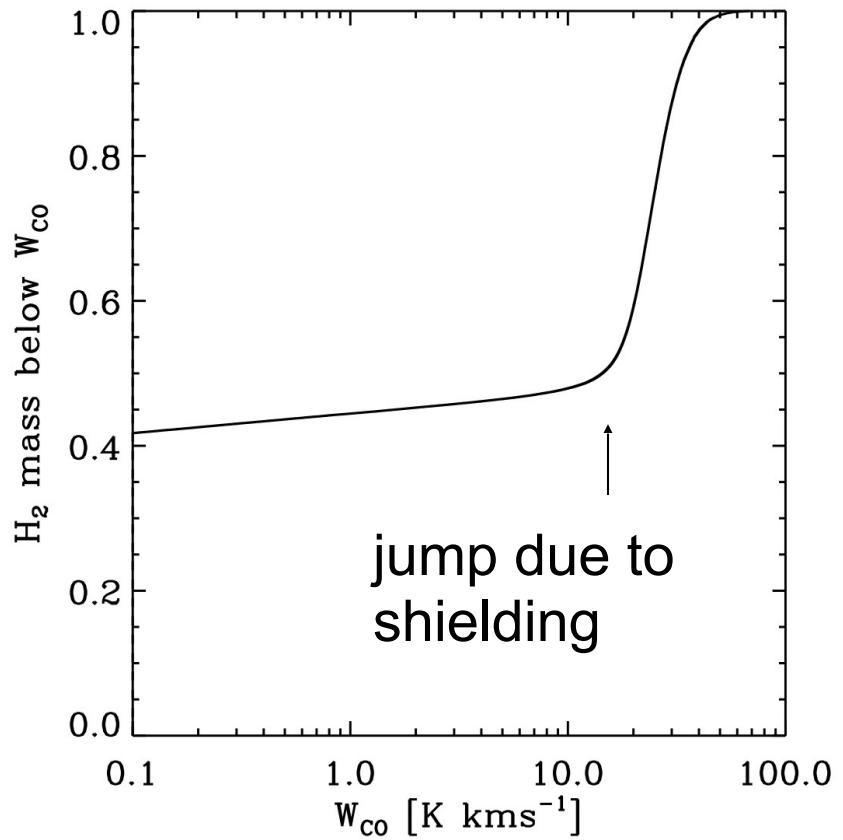
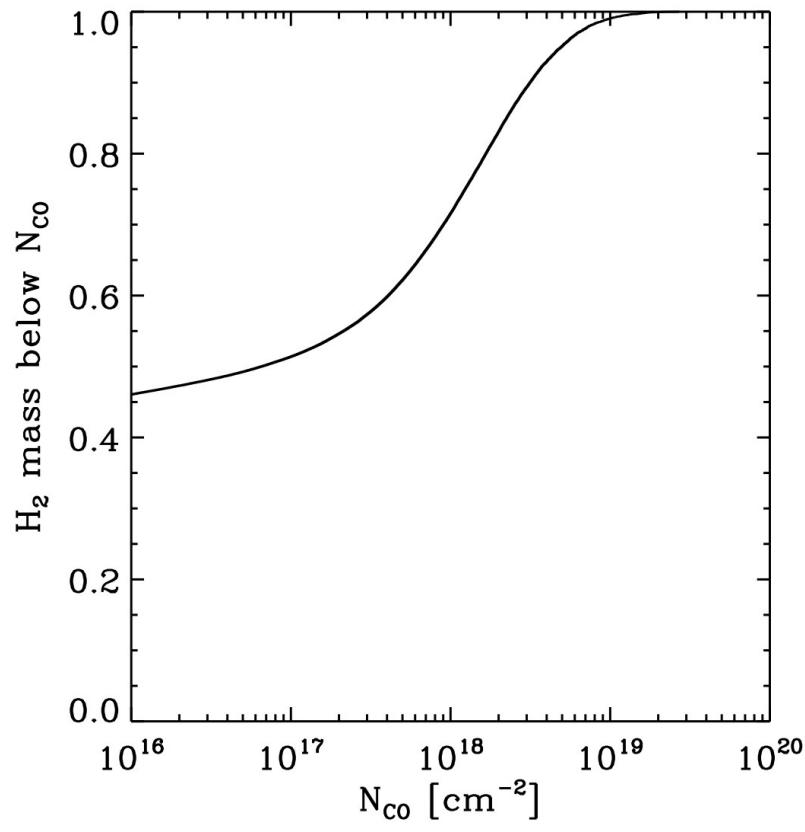


relation between CO and H₂



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}

$$f_{\text{DG}} = 0.42$$

$$X_{\text{CO}} = 2.2 \times 10^{20} \text{ cm}^{-2} \text{K}^{-1} \text{km}^{-1} \text{s}$$

dark gas fraction

Observational estimates:

Grenier et al. (2005) $f_{DG} = 0.33-0.5$

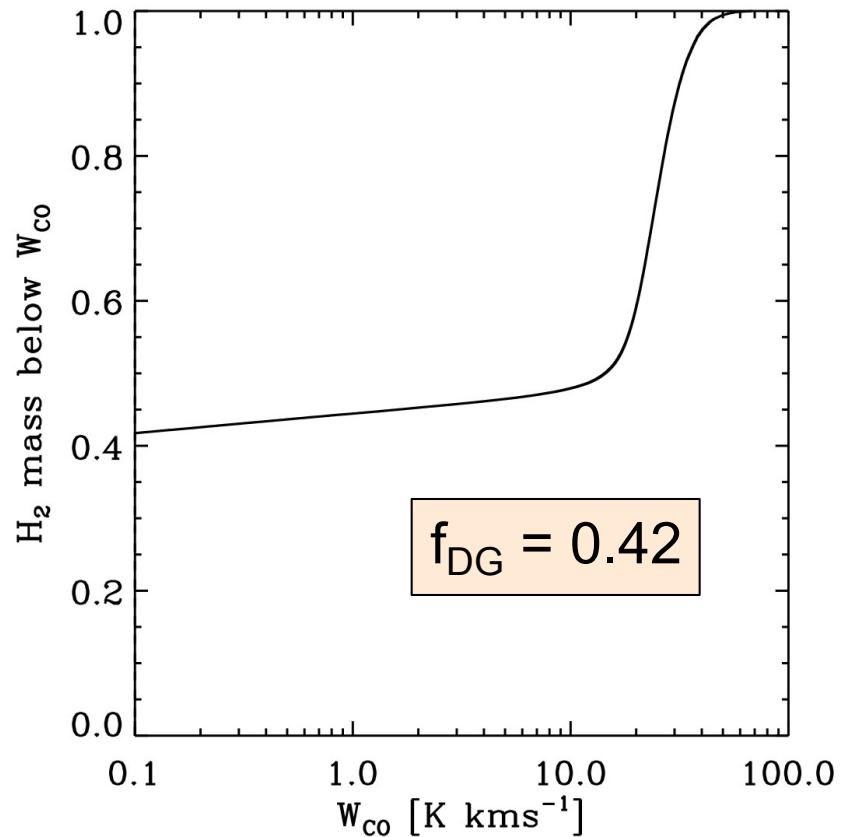
Planck coll. (2011)* $f_{DG} = 0.54$

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.) $f_{DG} \sim 0.5$

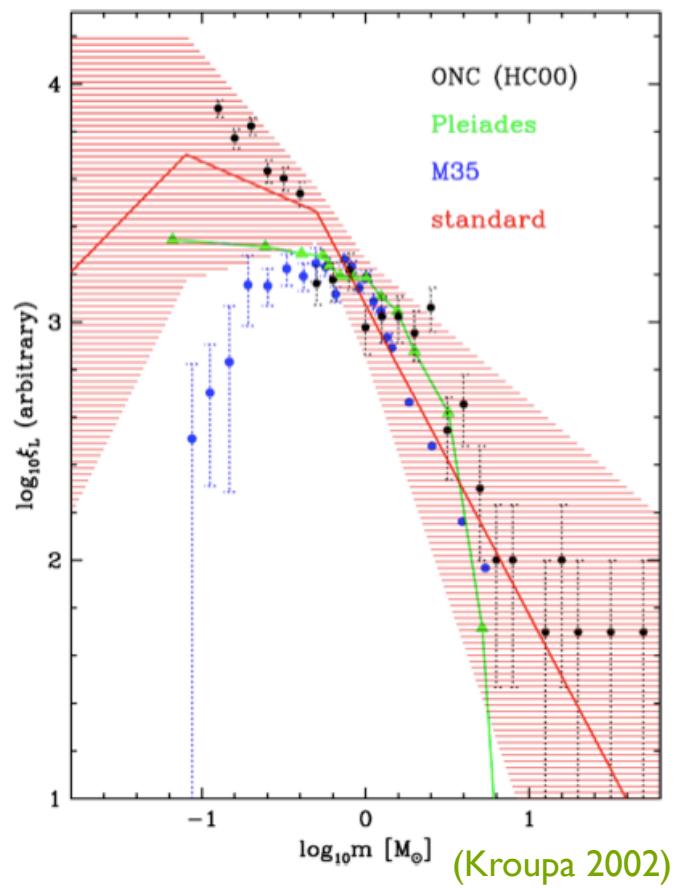


* dust methods have large uncertainties.

stellar mass
function

stellar mass function

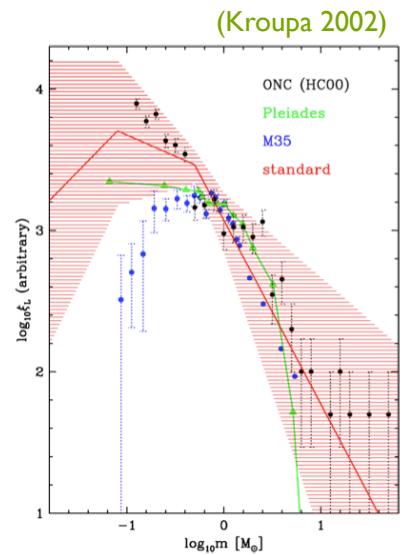
stars seem to follow a universal
mass function at birth --> IMF



Orion, NGC 3603, 30 Doradus
(Zinnecker & Yorke 2007)

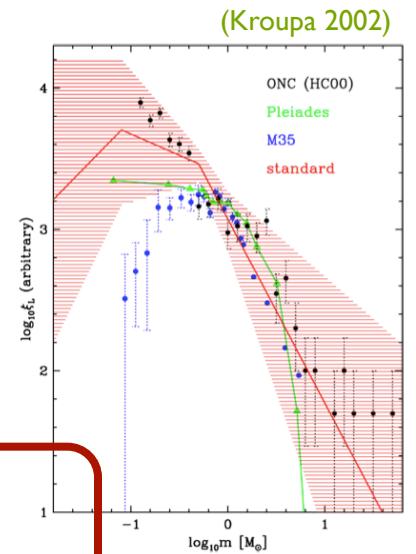
stellar mass function

- distribution of stellar masses depends on
 - turbulent initial conditions
--> mass spectrum of prestellar cloud cores
 - collapse and interaction of prestellar cores
--> accretion and N-body effects
 - thermodynamic properties of gas
--> balance between heating and cooling
--> EOS (determines which cores go into collapse)
 - (proto) stellar feedback terminates star formation
ionizing radiation, bipolar outflows, winds, SN, etc.



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application to early star formation

thermodynamics & fragmentation

degree of fragmentation depends on *EOS!*

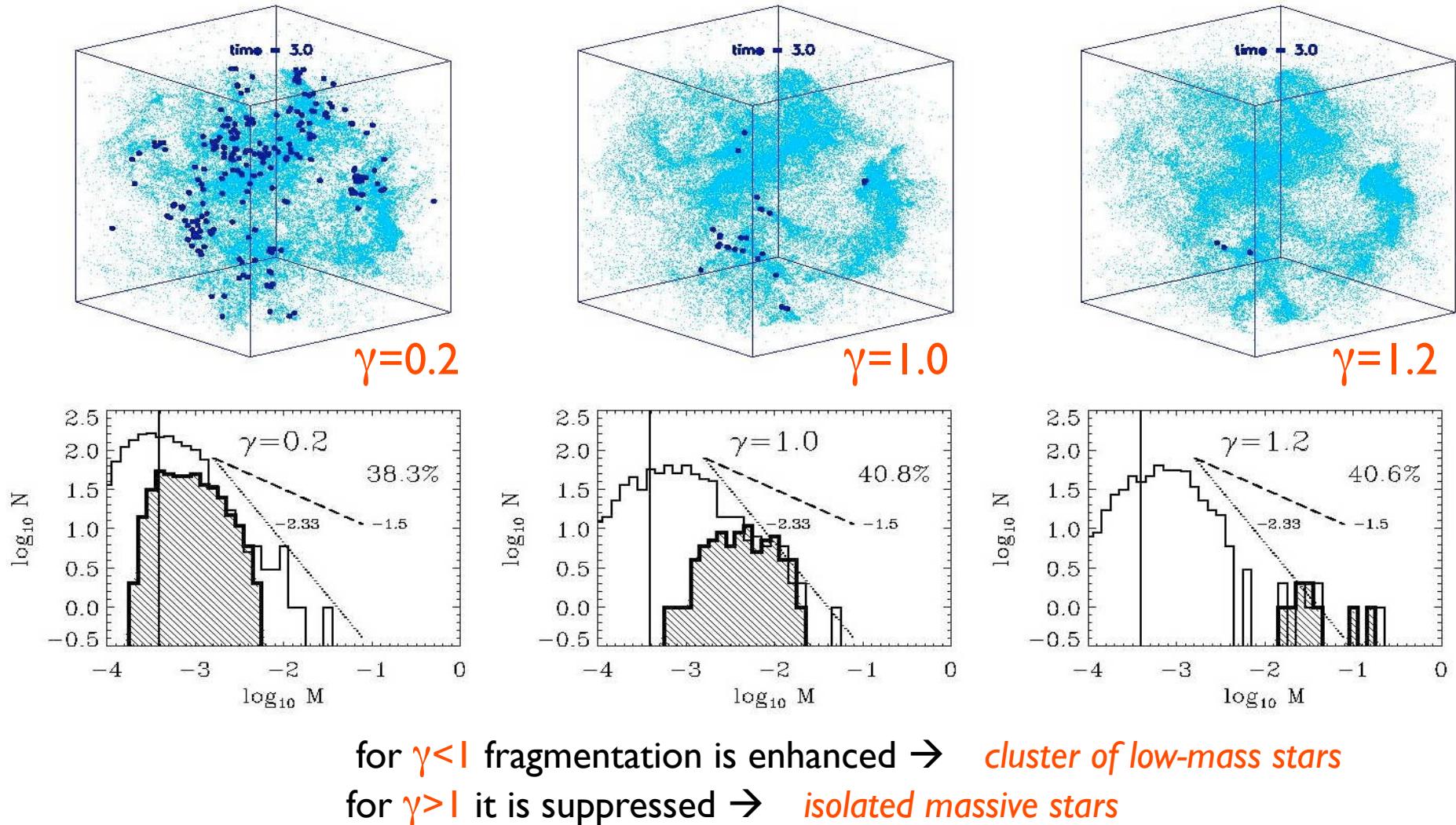
polytropic EOS: $p \propto \rho^\gamma$

$\gamma < 1$: dense cluster of low-mass stars

$\gamma > 1$: isolated high-mass stars

(see Li et al. 2003; also Kawachi & Hanawa 1998, Larson 2003)

dependency on EOS

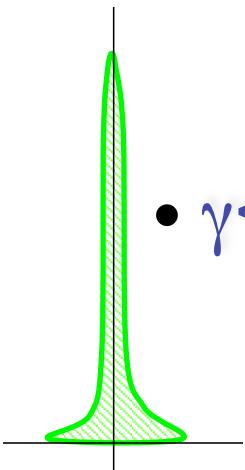


(from Li, Klessen, & Mac Low 2003, ApJ, 592, 975)

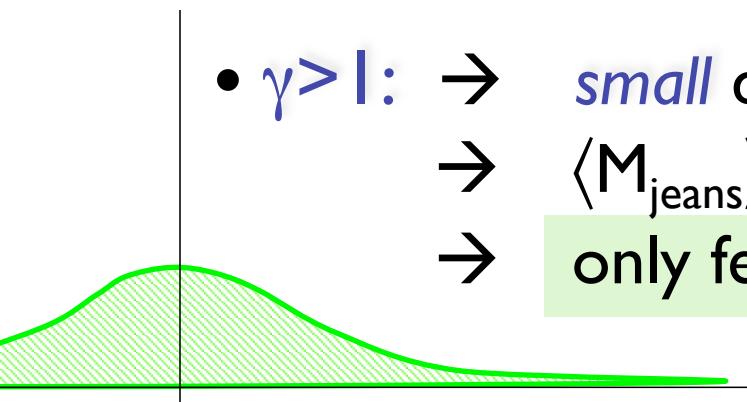
how does that work?

$$(1) \ p \propto \rho^\gamma \rightarrow \rho \propto p^{1/\gamma}$$

$$(2) \ M_{\text{jeans}} \propto \gamma^{3/2} p^{(3\gamma-4)/2}$$

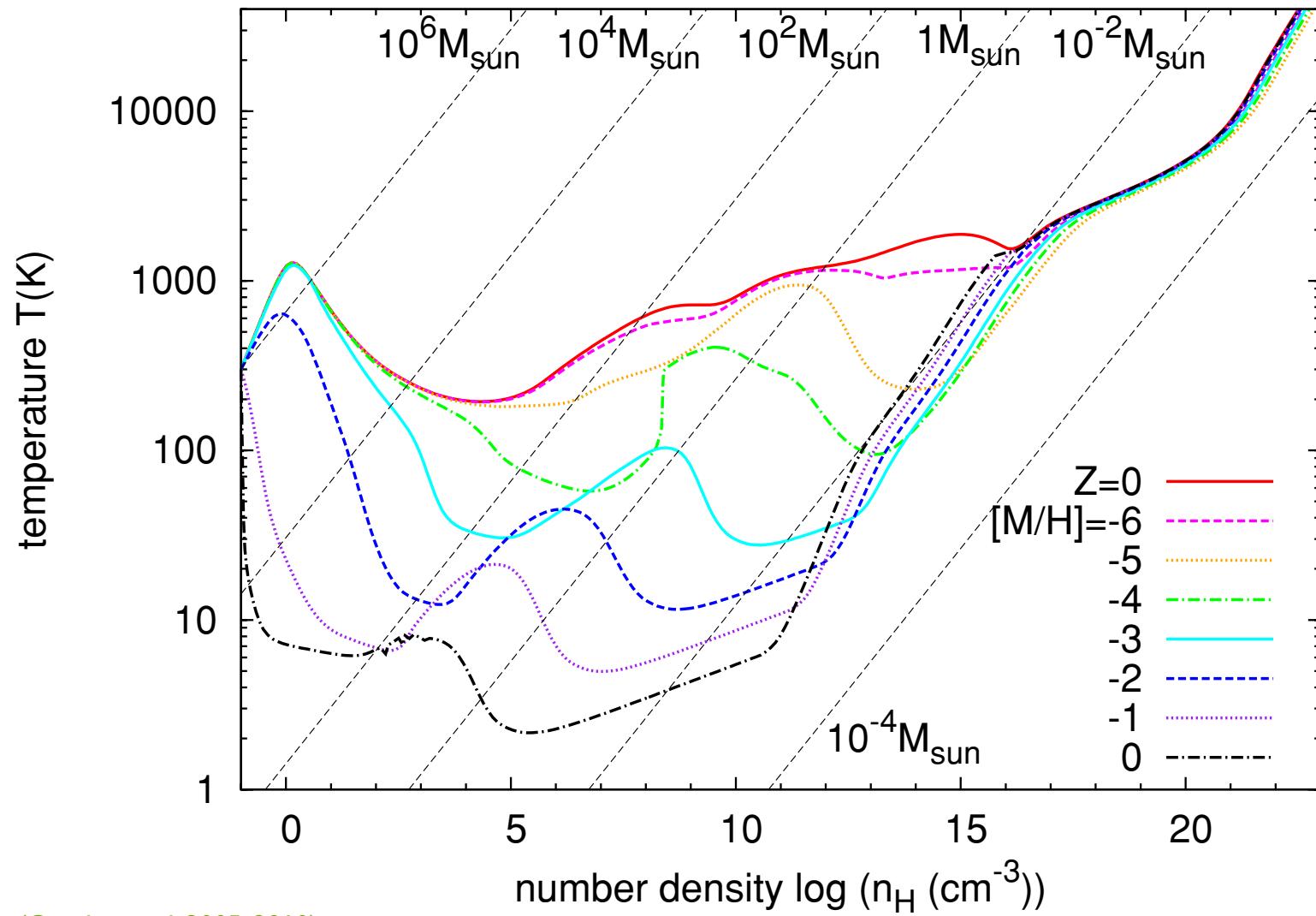


- $\gamma < 1$:
→ *large* density excursion for given pressure
→ $\langle M_{\text{jeans}} \rangle$ becomes small
→ number of fluctuations with $M > M_{\text{jeans}}$ is large



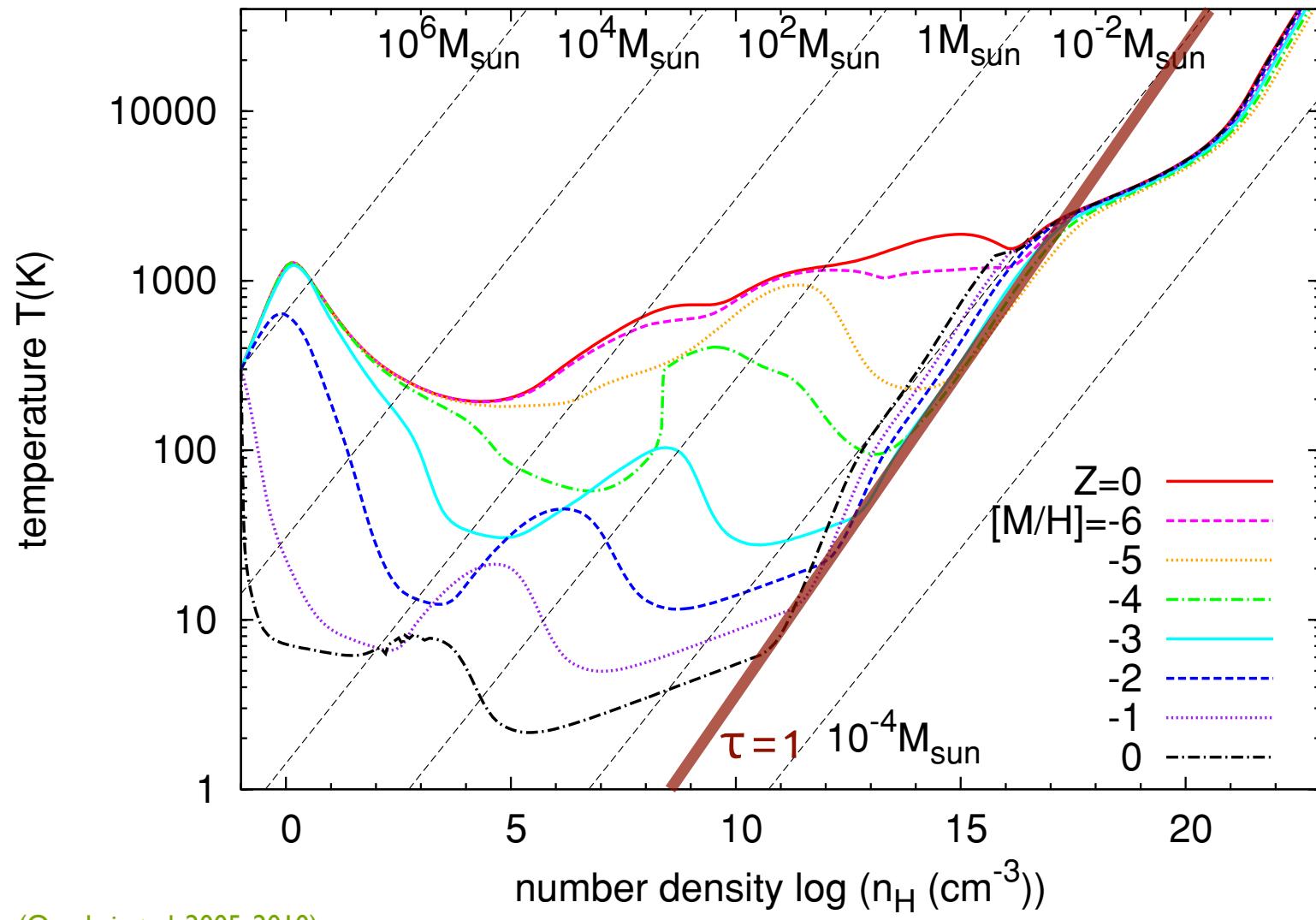
- $\gamma > 1$:
→ *small* density excursion for given pressure
→ $\langle M_{\text{jeans}} \rangle$ is large
→ only few and massive clumps exceed M_{jeans}

EOS as function of metallicity



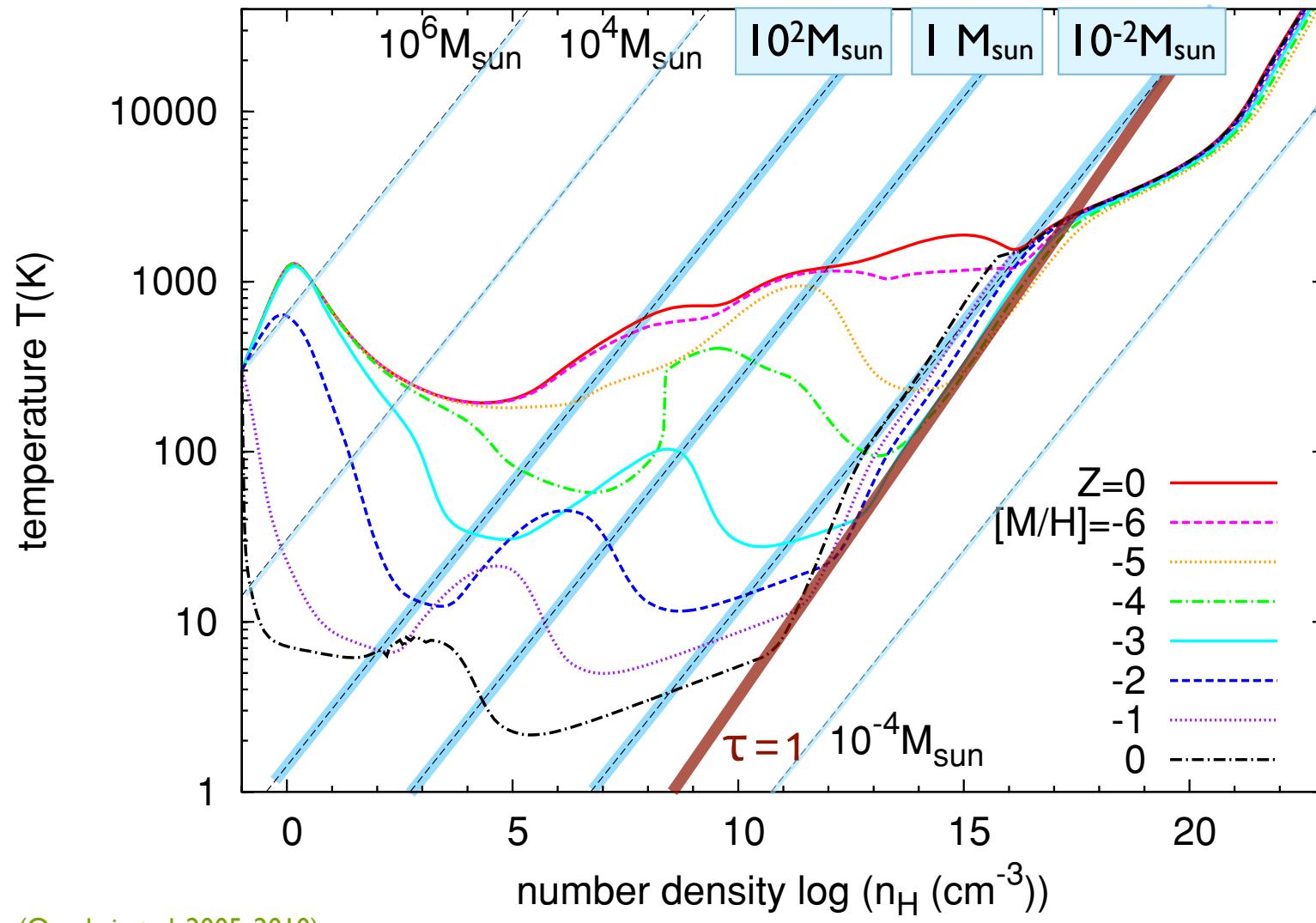
(Omukai et al. 2005, 2010)

EOS as function of metallicity



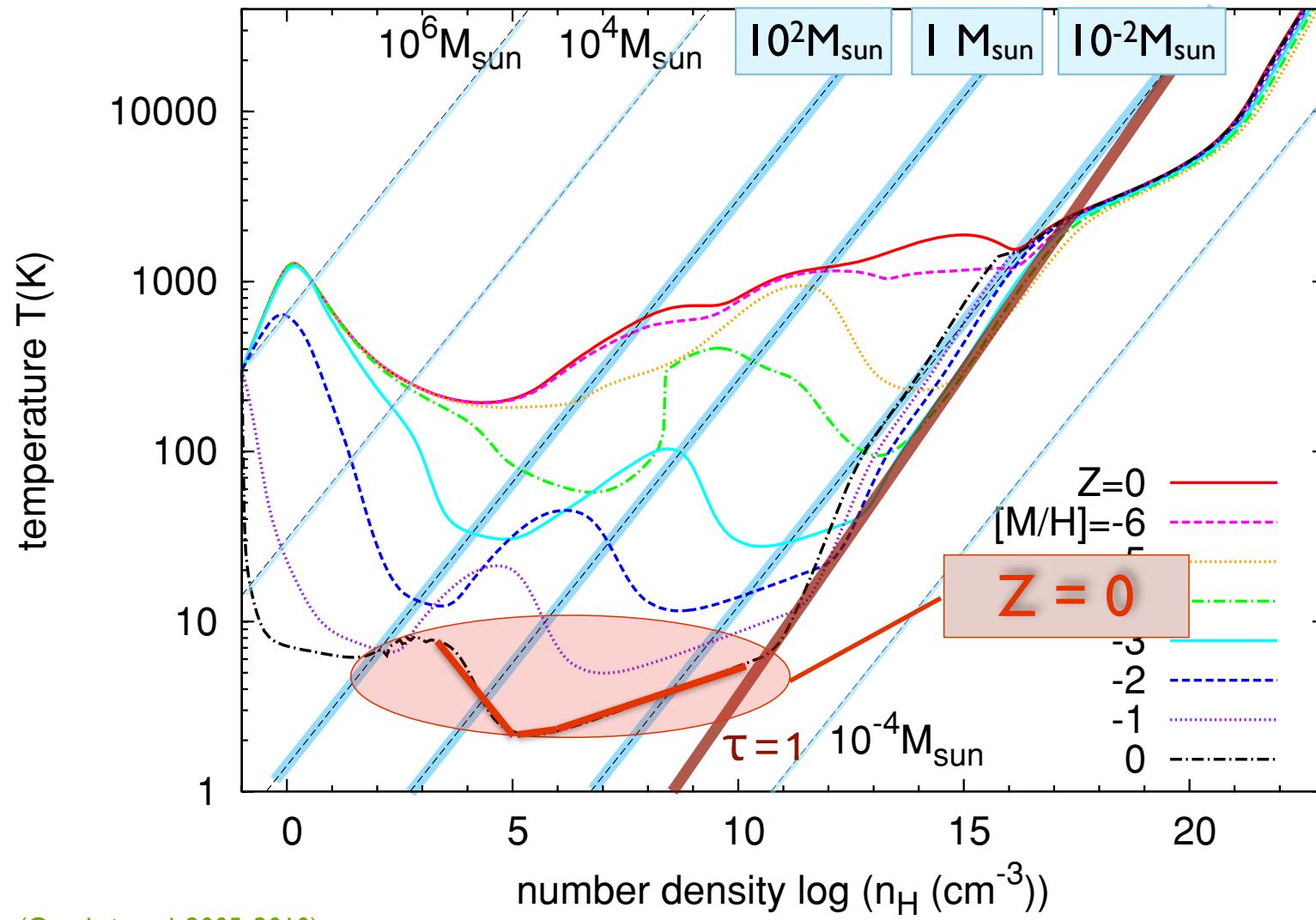
(Omukai et al. 2005, 2010)

EOS as function of metallicity



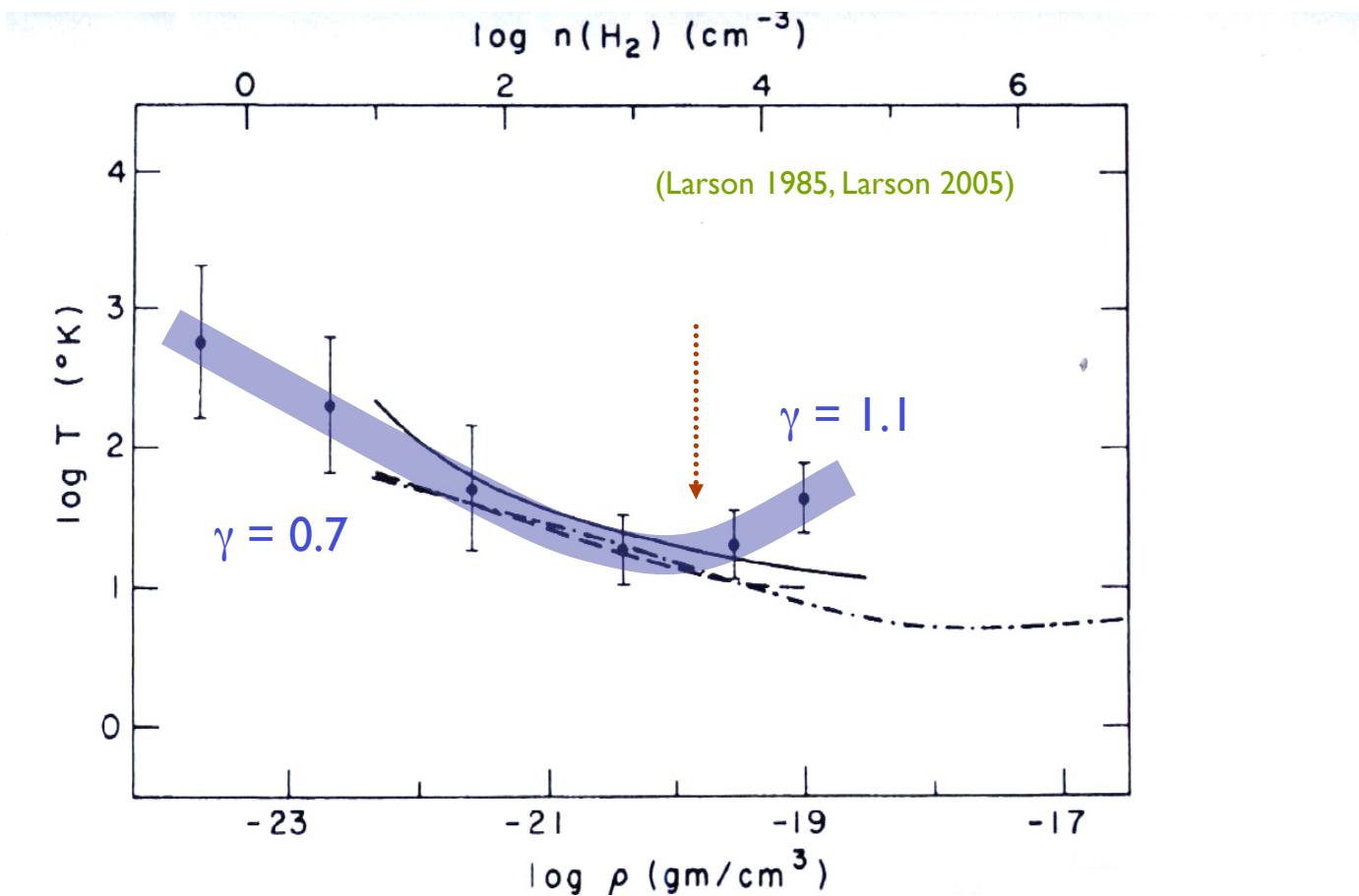
(Omukai et al. 2005, 2010)

EOS as function of metallicity

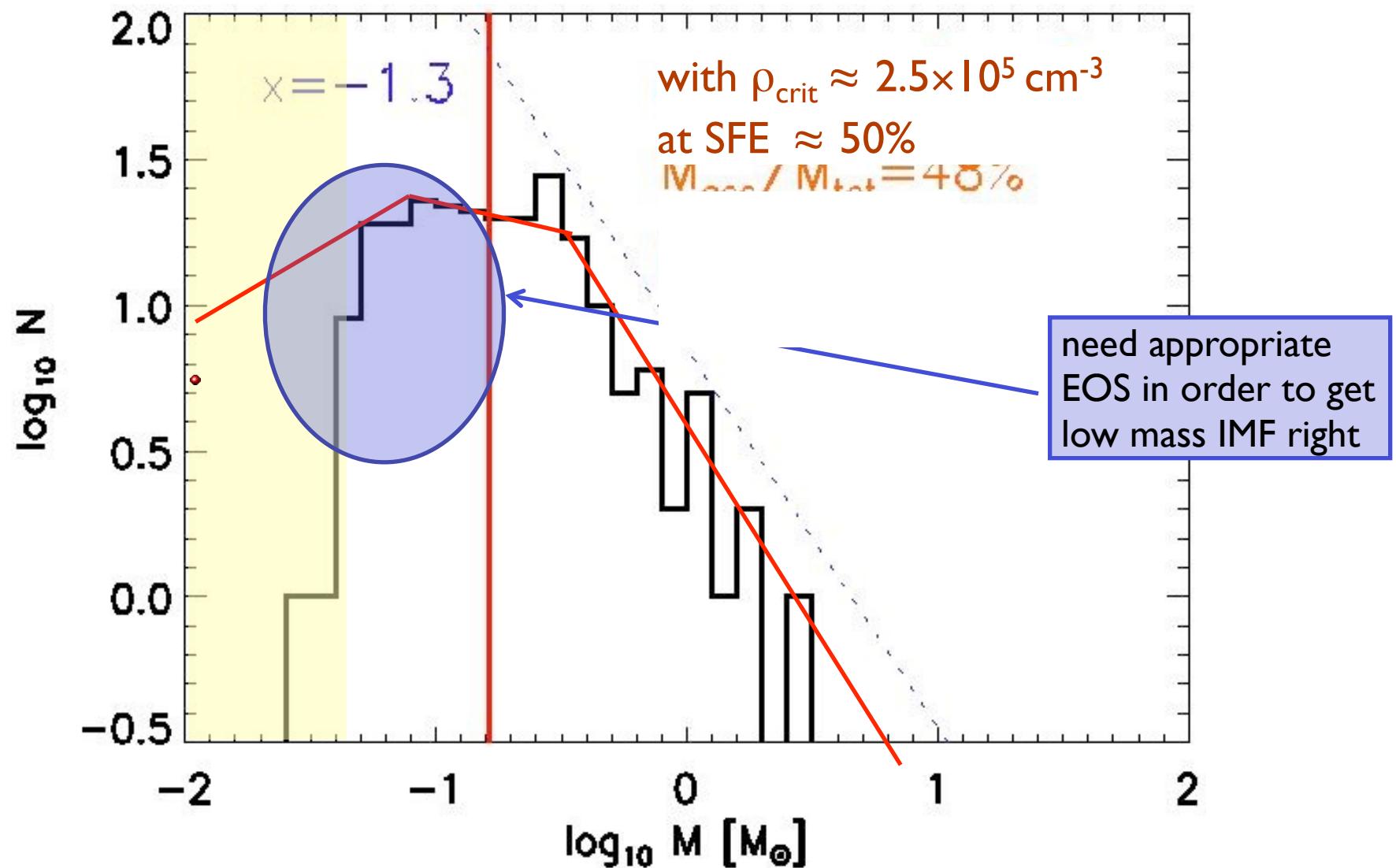


(Omukai et al. 2005, 2010)

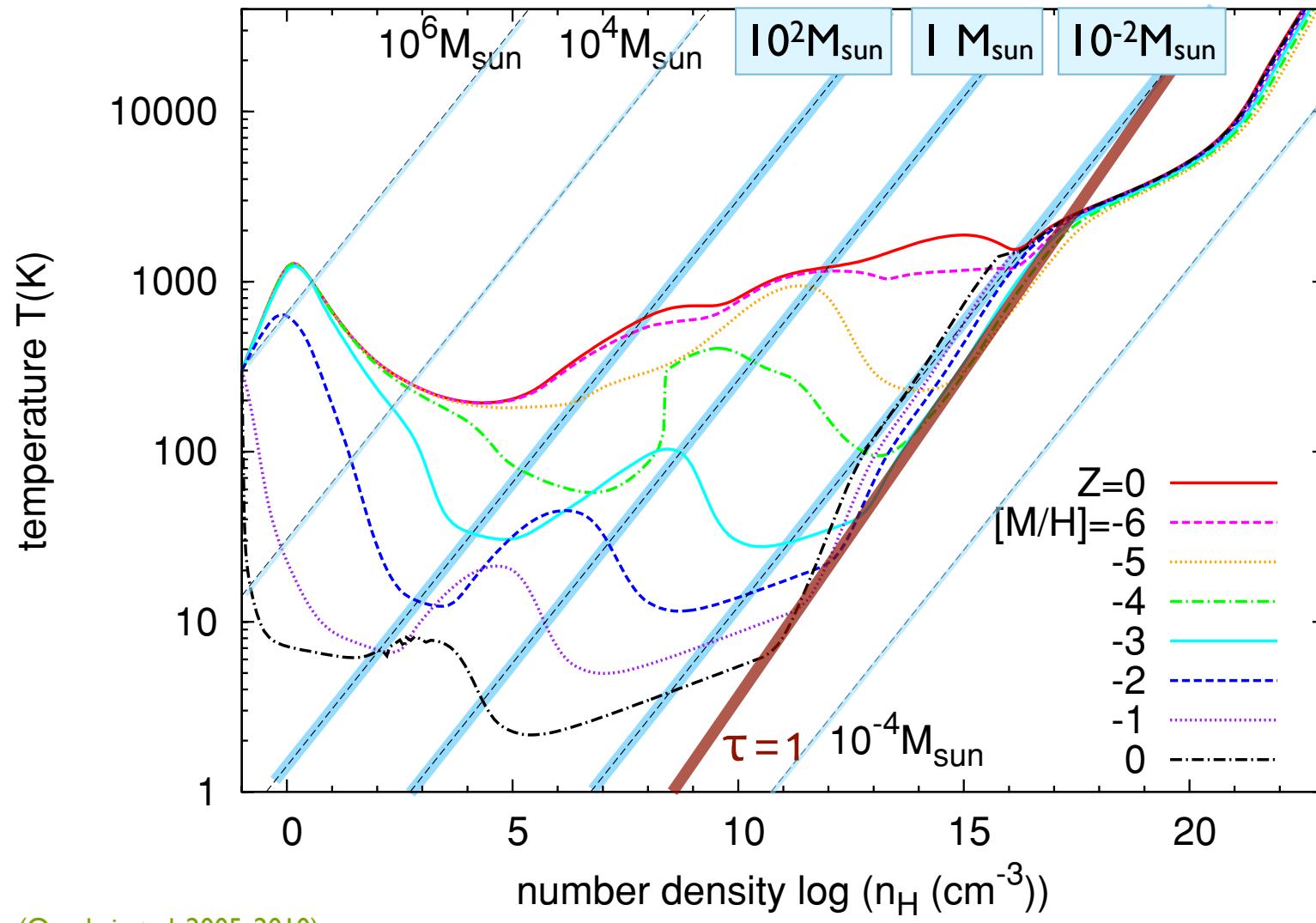
present-day star formation



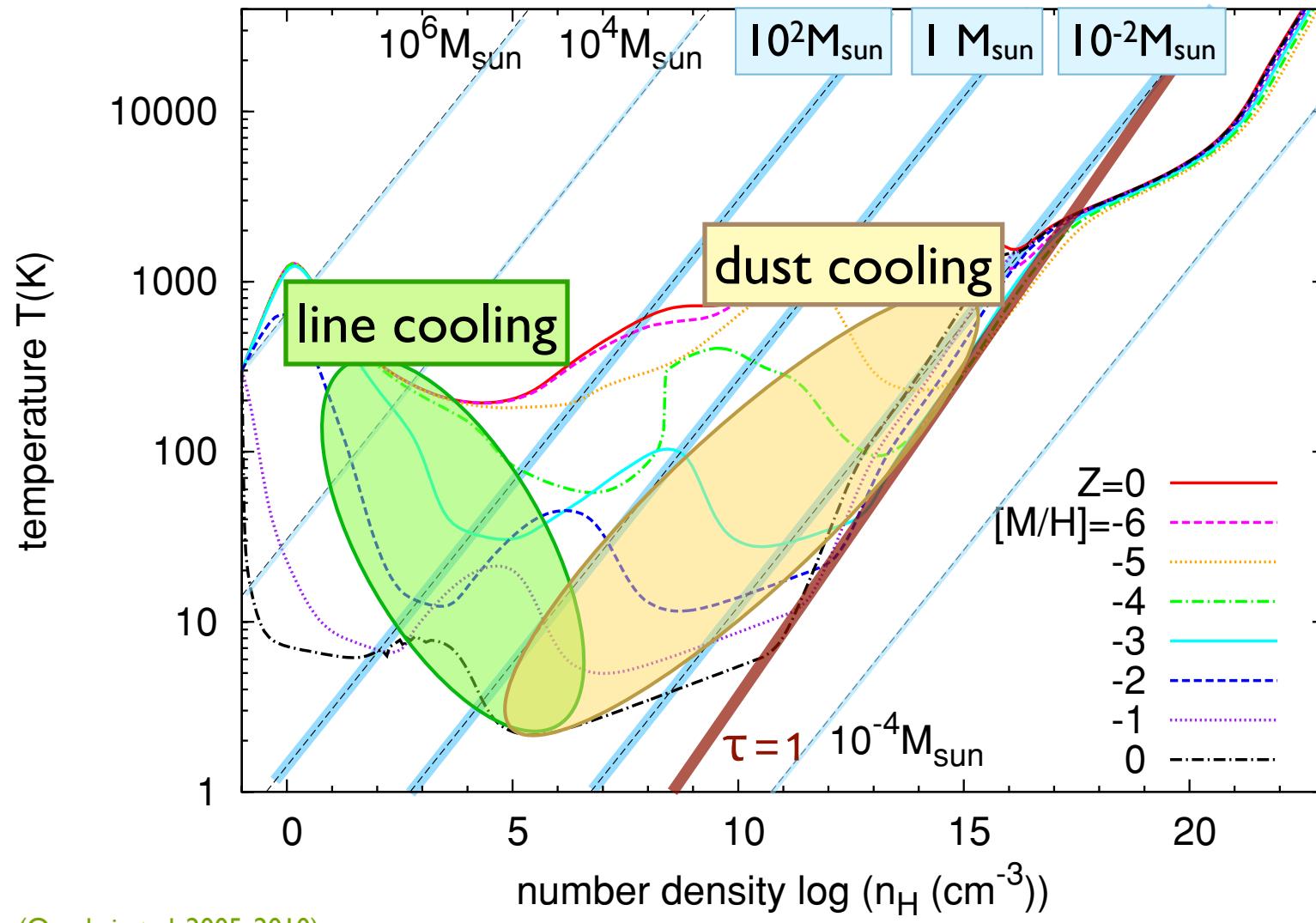
IMF in nearby molecular clouds



EOS as function of metallicity

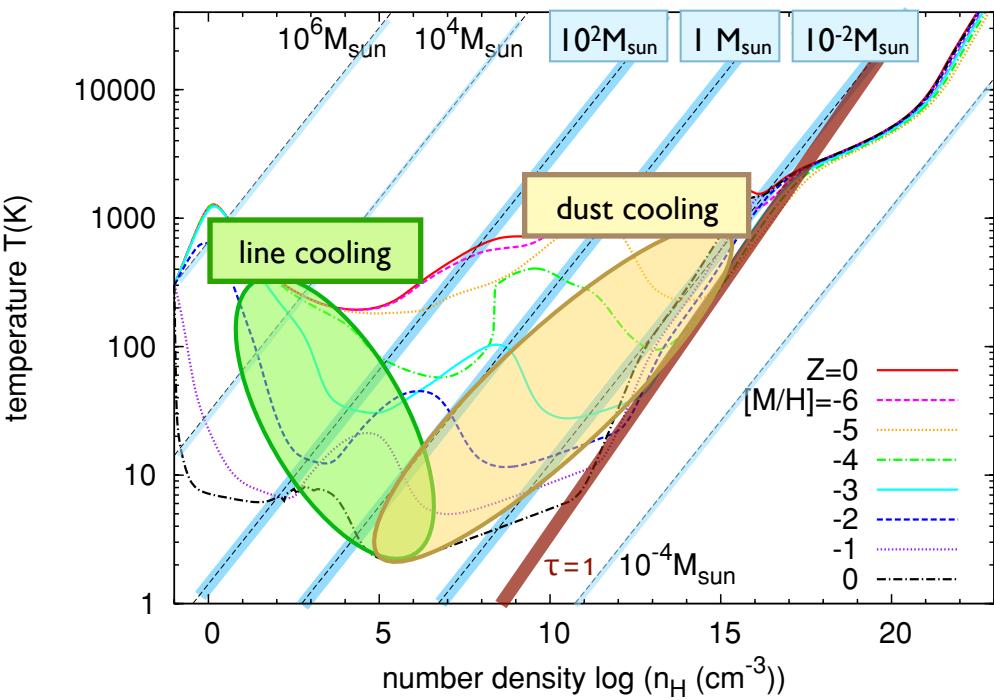


EOS as function of metallicity



(Omukai et al. 2005, 2010)

transition: Pop III to Pop II.5

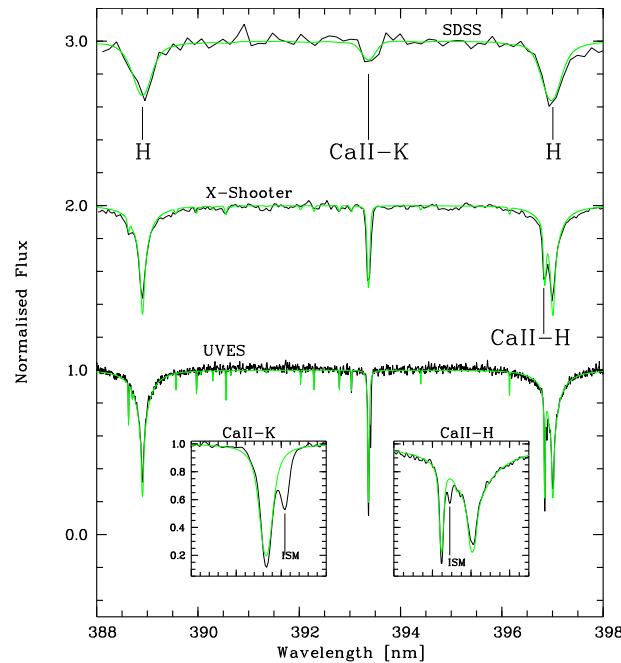


two competing models:

- cooling due to atomic fine-structure lines ($Z > 10^{-3.5} Z_{\text{sun}}$)
- cooling due to coupling between gas and dust ($Z > 10^{-5...-6} Z_{\text{sun}}$)
- which one explains origin of extremely metal-poor stars?
NB: lines would only make very massive stars, with $M > \text{few } \times 10 M_{\text{sun}}$.

(Omukai et al. 2005, 2010)

transition: Pop III to Pop II.5



SDSS J1029151+172927

- is first ultra metal-poor star with $Z \sim 10^{-4.5} Z_{\text{sun}}$ for all metals seen (Fe, C, N, etc.)
[see Caffau et al. 2011]
- this is in regime, where metal-lines cannot provide cooling
[e.g. Schneider et al. 2011, 2012, Klessen et al. 2012]

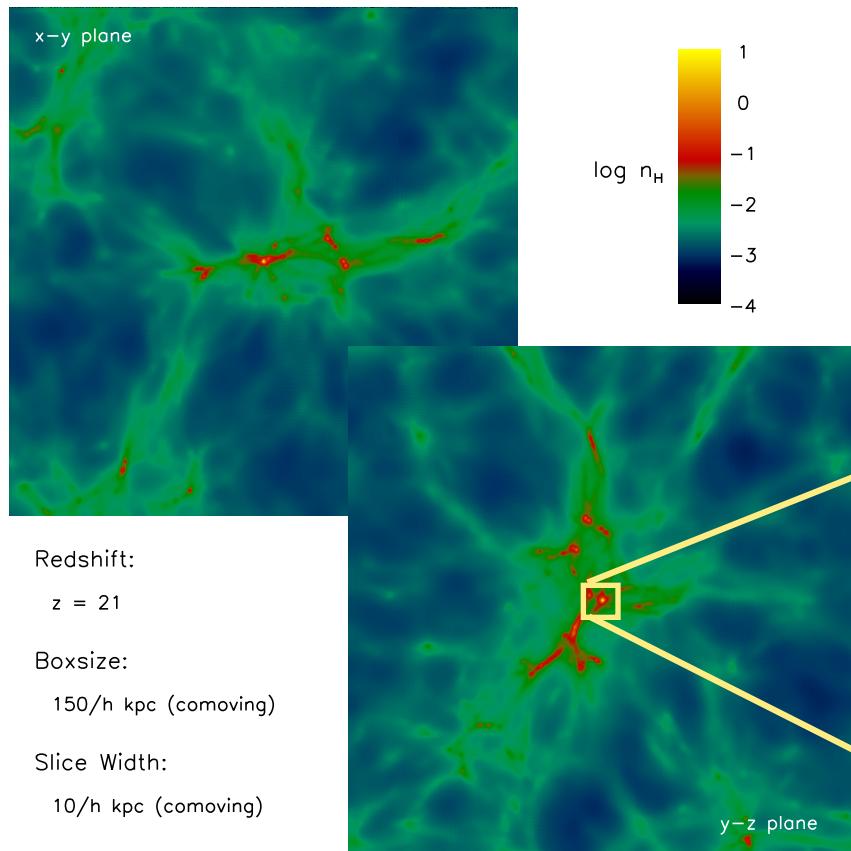
Element		$[X/H]_{\text{ID}}$		N lines	S_H	$A(X)_{\odot}$
	+3Dcor.	+NLTE cor.	+ 3D cor + NLTE cor			
C	≤ -3.8	≤ -4.5		G-band	8.50	
N	≤ -4.1	≤ -5.0		NH-band	7.86	
Mg I	-4.71 ± 0.11	-4.68 ± 0.11	-4.52 ± 0.11	-4.49 ± 0.12	5	7.54
Si I	-4.27	-4.30	-3.93	-3.96	1	7.52
Ca I	-4.72	-4.82	-4.44	-4.54	1	6.33
Ca II	-4.81 ± 0.11	-4.93 ± 0.03	-5.02 ± 0.02	-5.15 ± 0.09	3	6.33
Ti II	-4.75 ± 0.18	-4.83 ± 0.16	-4.76 ± 0.18	-4.84 ± 0.16	6	4.90
Fe I	-4.73 ± 0.13	-5.02 ± 0.10	-4.60 ± 0.13	-4.89 ± 0.10	43	7.52
Ni II	-4.55 ± 0.14	-4.90 ± 0.11		10	6.23	
Sr II	≤ -5.10	≤ -5.25	≤ -4.94	≤ -5.09	1	2.92

(Caffau et al. 2011, 2012)

• TOPoS ESO large program to find more of these stars (120h x-shooter, 30h UVES)
(Caffau et al. 2013, A&A, 560, A71, Bonifacio et al. 2014, in prep)

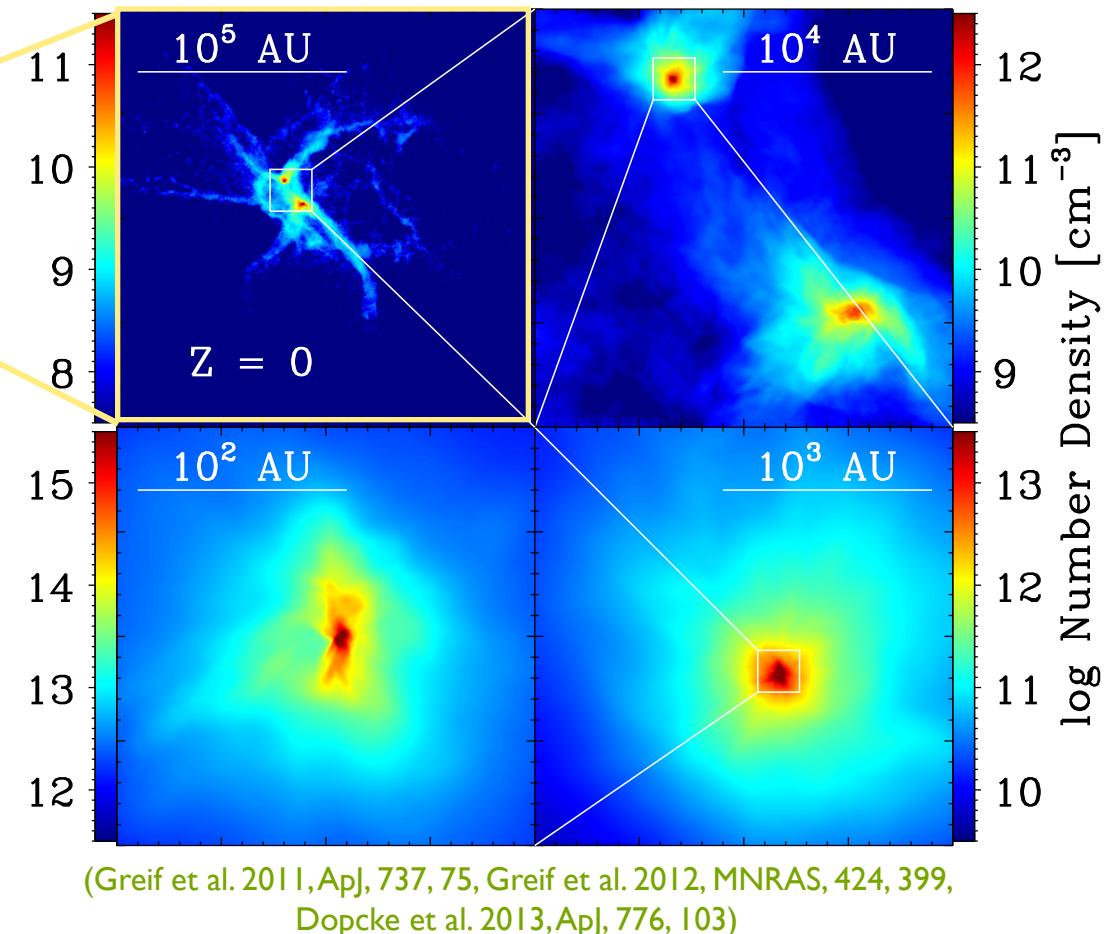
(Schneider et al. 2011, 2012, Klessen et al. 2012)

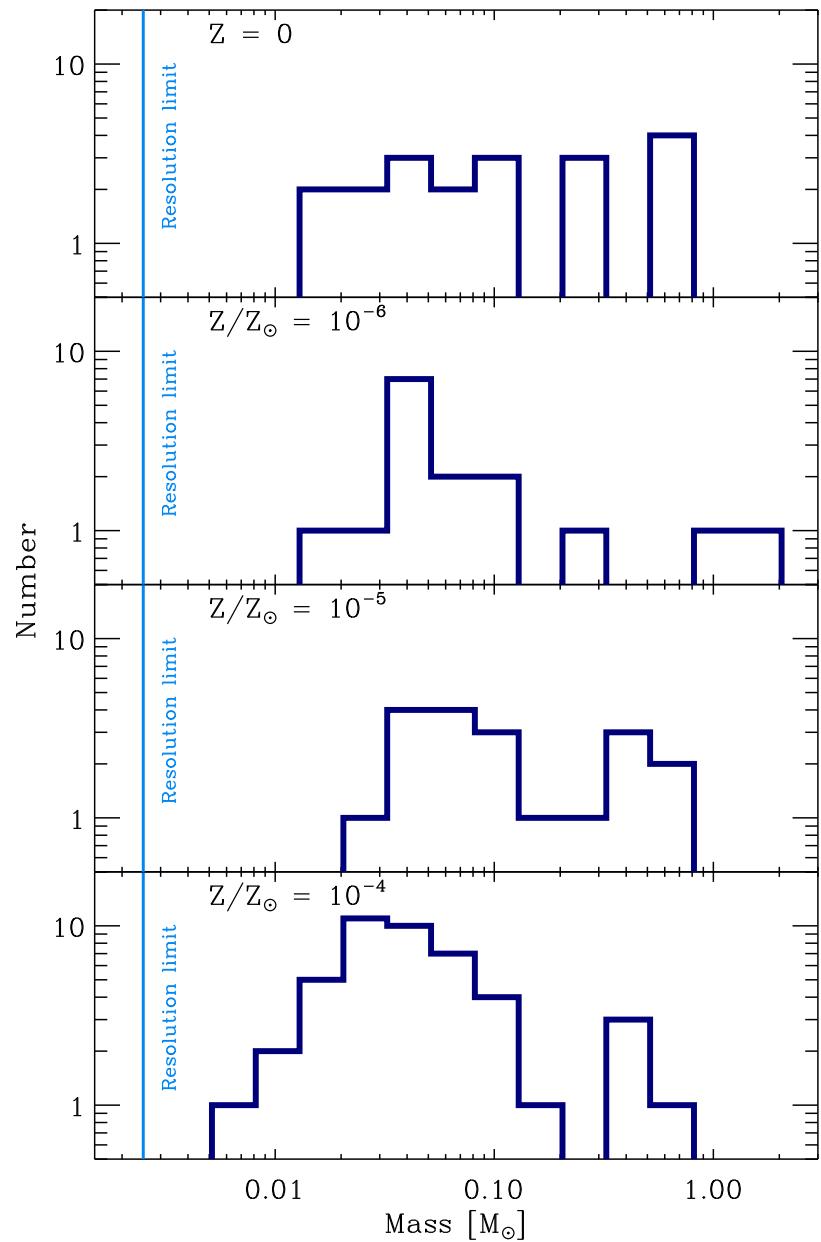
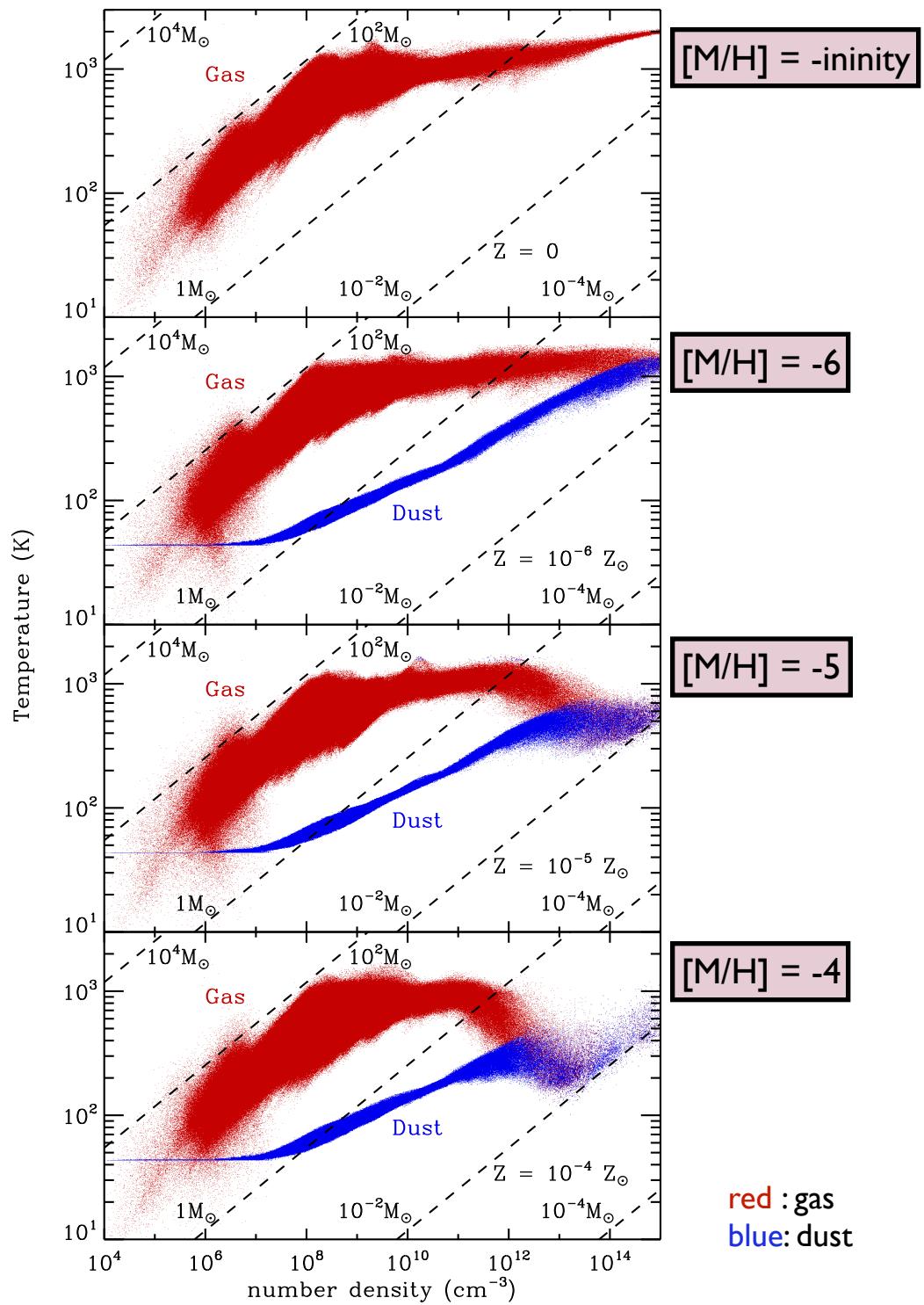
modeling the formation of the first/second stars



(Greif et al., 2007, ApJ, 670, 1)

successive zoom-in calculation from cosmological initial conditions (using SPH and new grid-code AREPO)

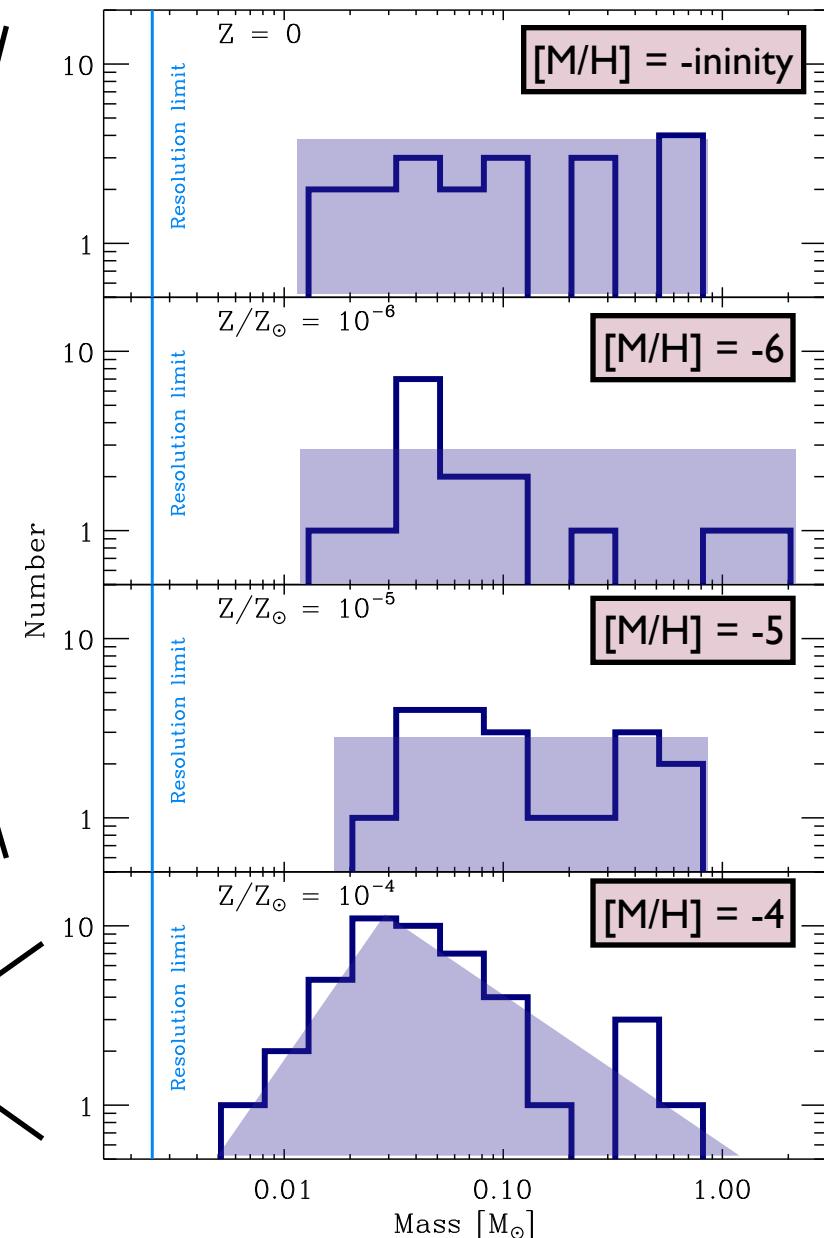




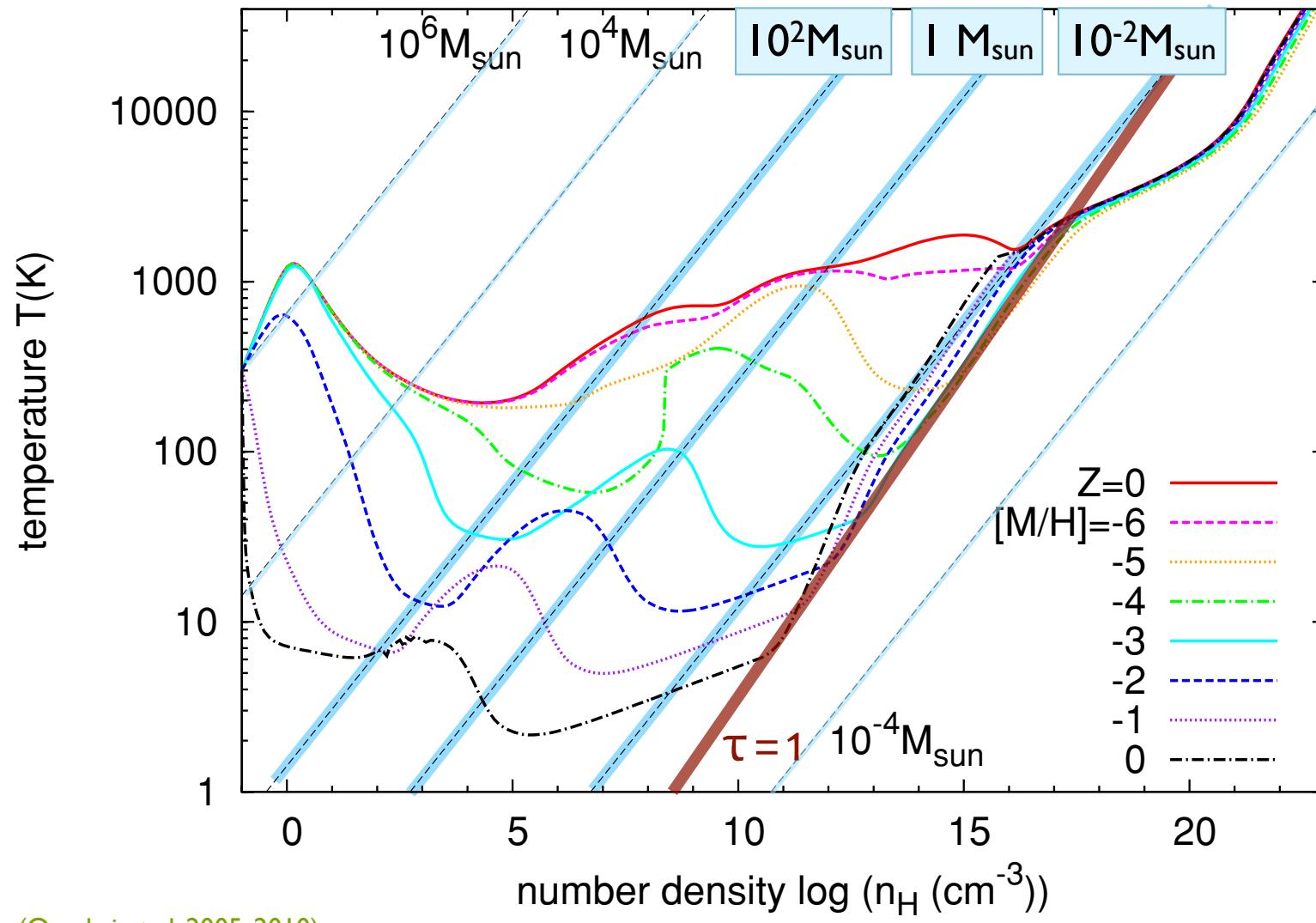
hints for differences
in mass spectrum

disk fragmentation mode

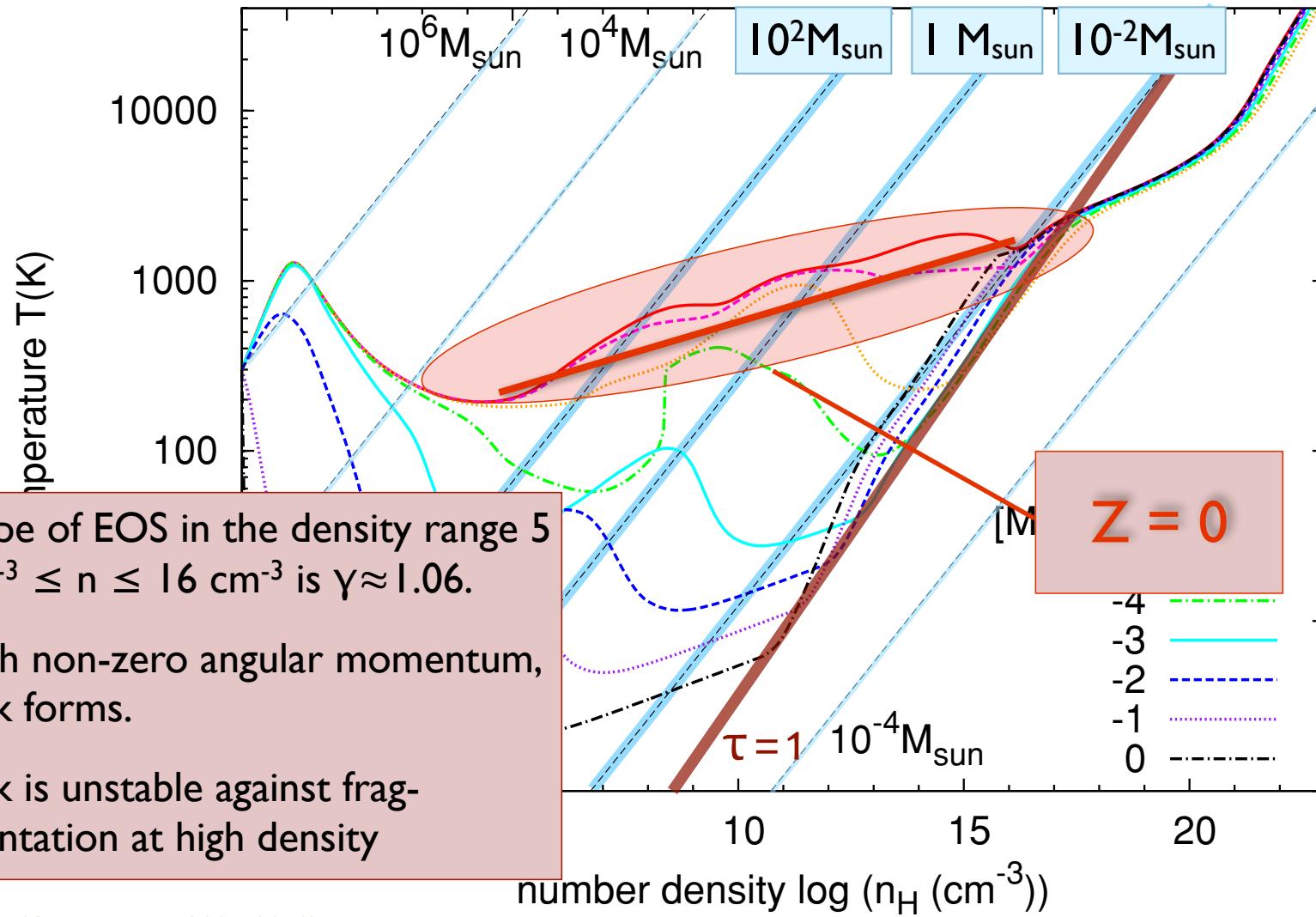
gravoturbulent fragmentation mode



EOS as function of metallicity



EOS as function of metallicity



detailed look at accretion disk

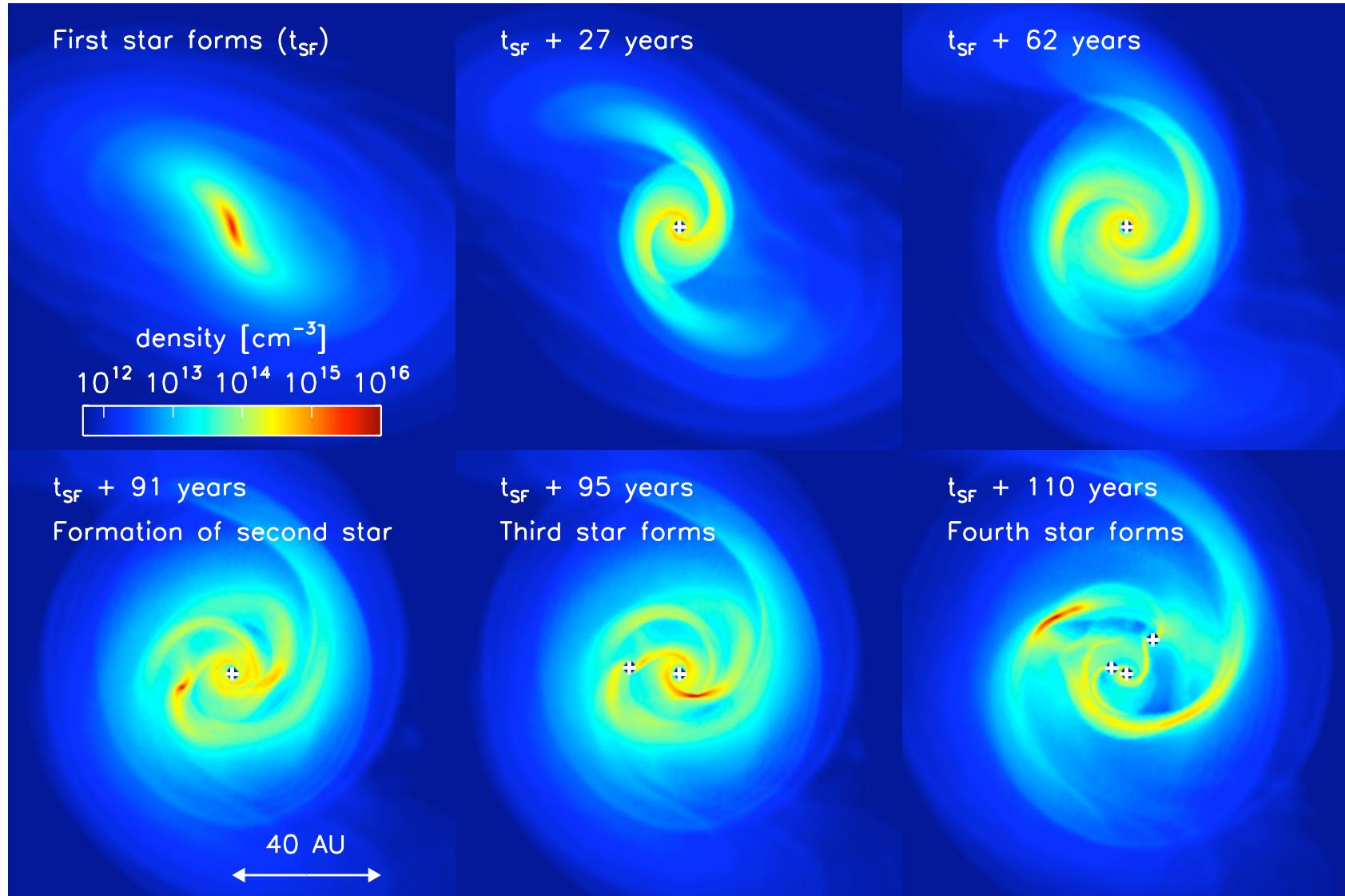
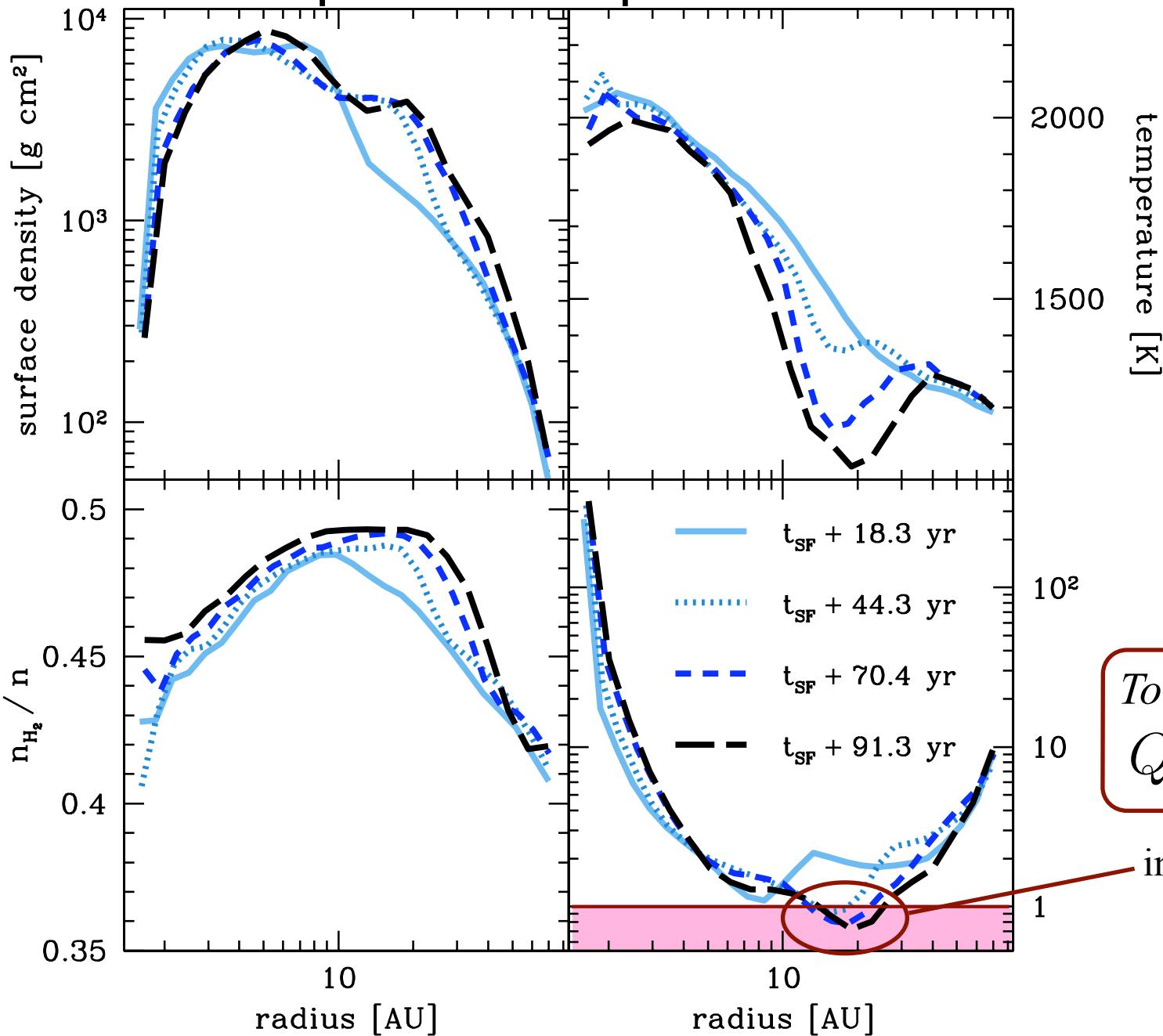


Figure 1: Density evolution in a 120 AU region around the first protostar, showing the build-up of the protostellar disk and its eventual fragmentation. We also see ‘wakes’ in the low-density regions, produced by the previous passage of the spiral arms.

important disk parameters

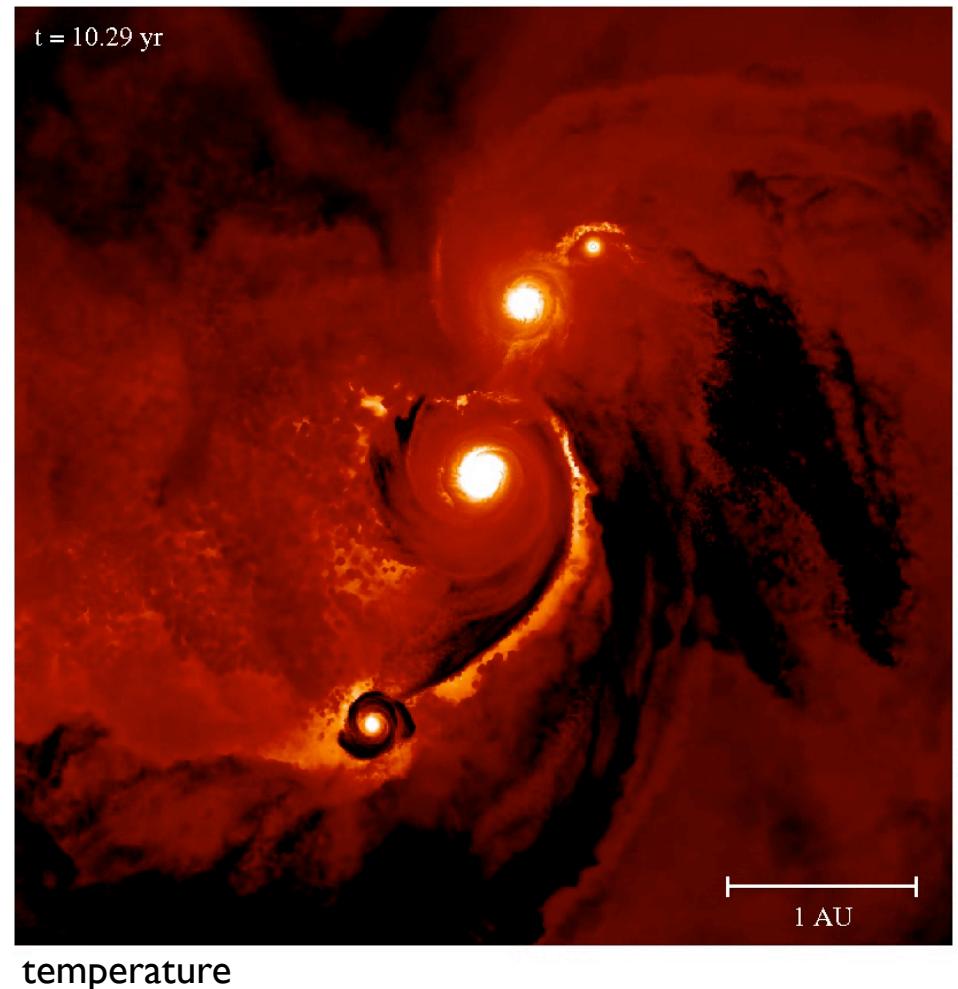
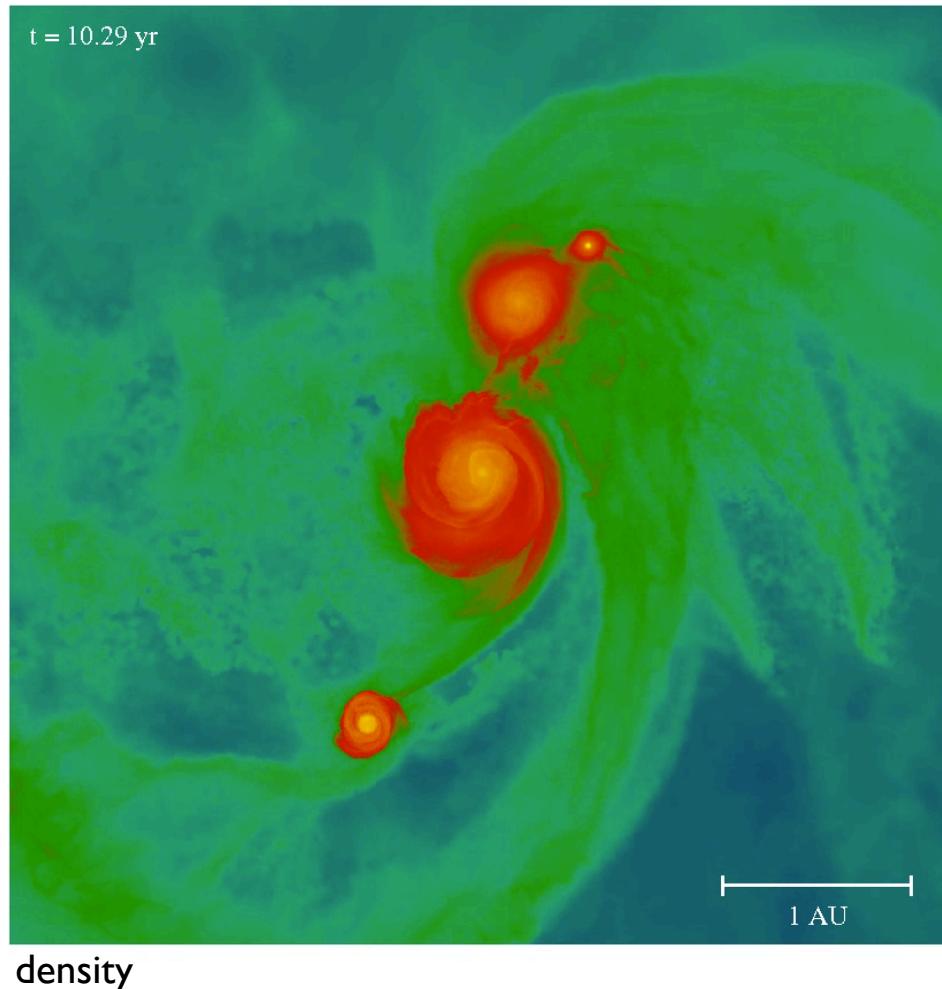


Toomre Q :

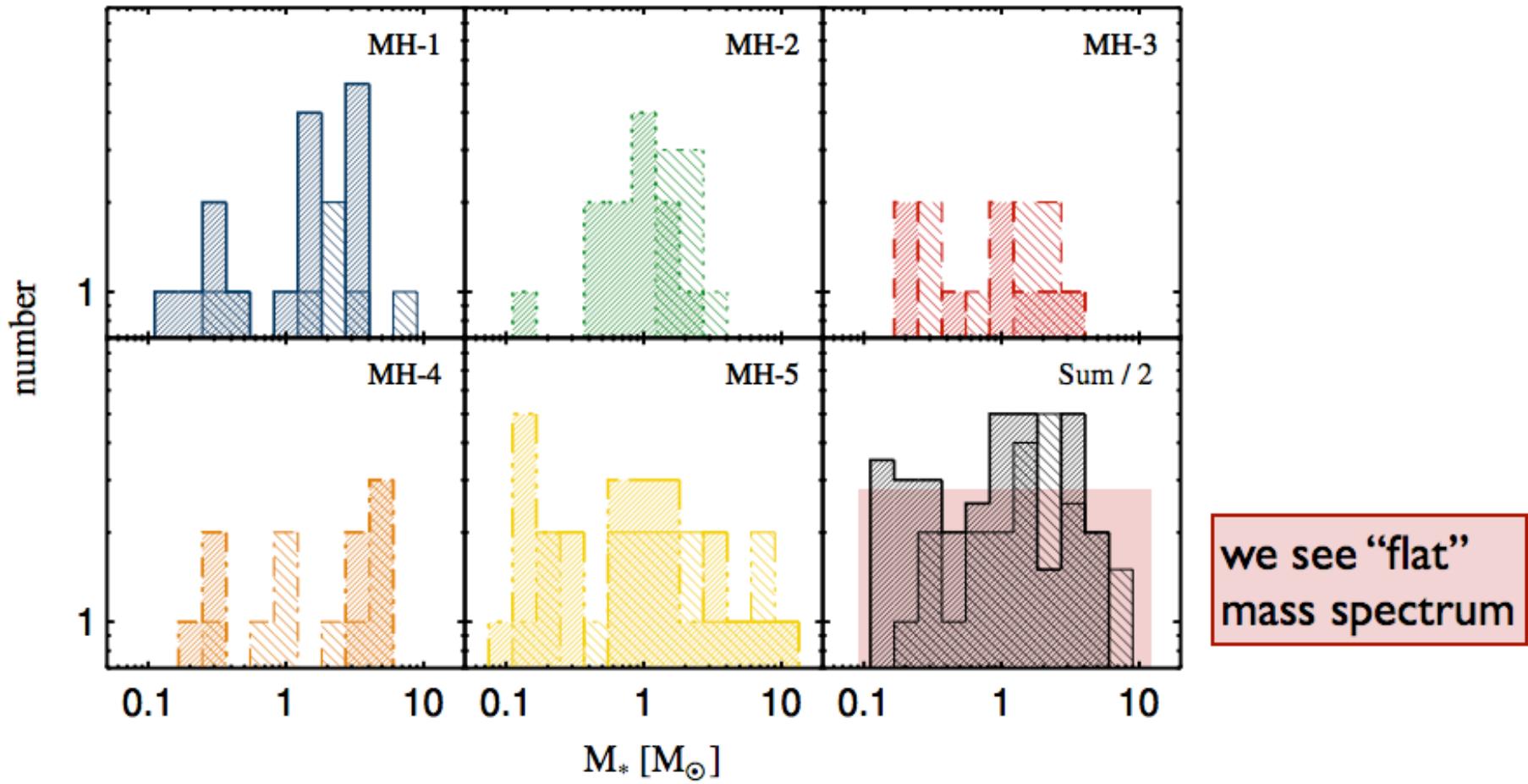
$$Q = c_s \kappa / \pi G \Sigma$$

instability for $Q < 1$

Most recent calculations:
fully sink-less simulations, following the disk build-up over ~ 10 years
(resolving the protostars - first cores - down to 10^5 km $\sim 0.01 R_\odot$)

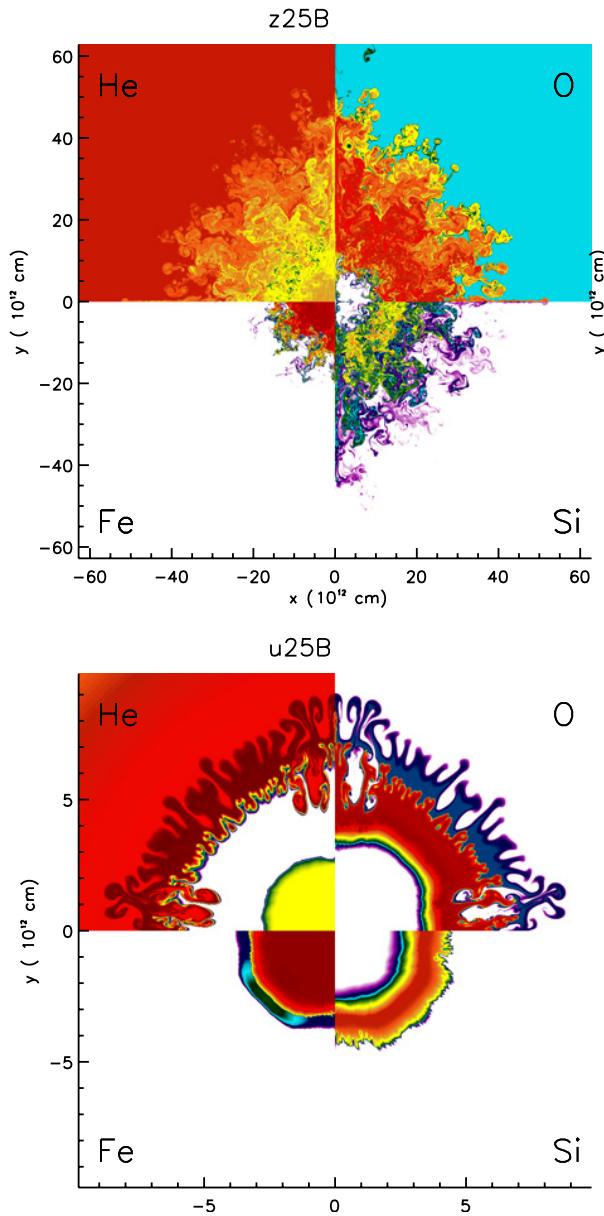


expected mass spectrum

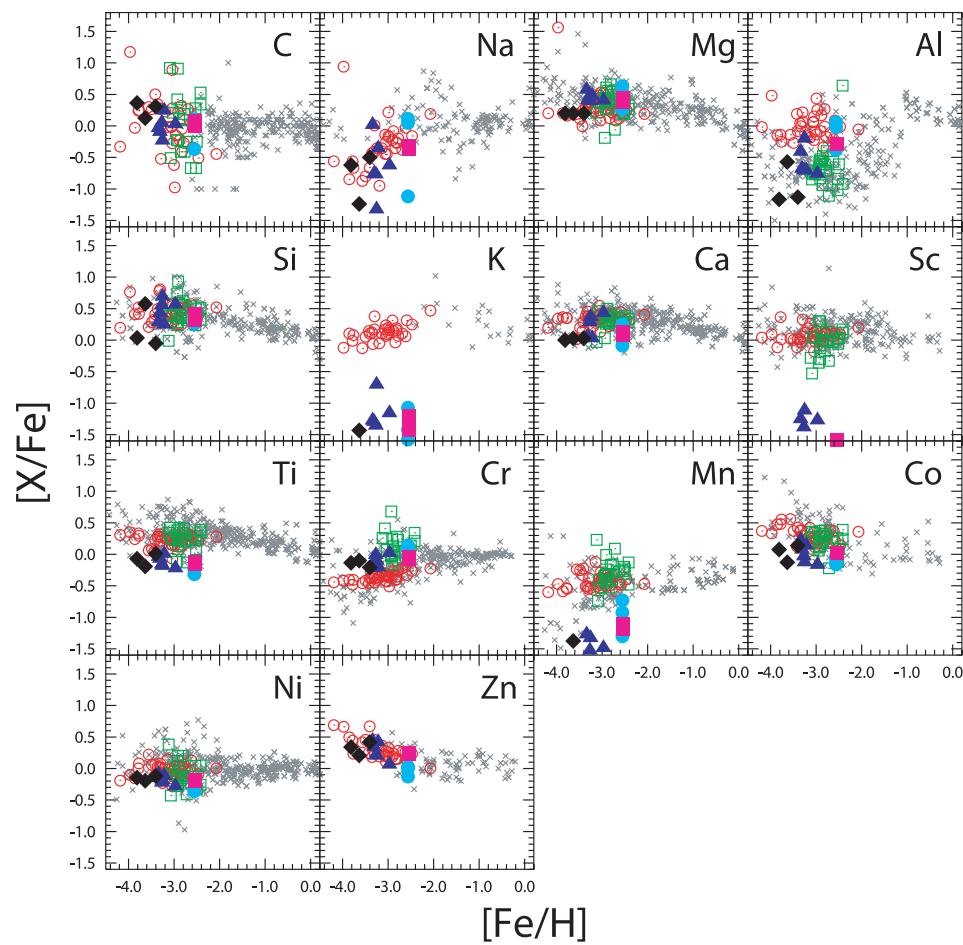


expected mass spectrum

- expected IMF is flat and covers a wide range of masses
- implications
 - because slope > -2 , most mass is in massive objects as predicted by most previous calculations
 - most high-mass Pop III stars should be in *binary systems*
--> source of *high-redshift gamma-ray bursts*
 - because of ejection, some *low-mass objects* ($< 0.8 M_{\odot}$) might have survived until today and could potentially be found in the Milky Way
- consistent with abundance patterns found in second generation stars



(Joggerst et al. 2009, 2010)



(Tominaga et al. 2007)

The metallicities of extremely metal-poor stars in the halo are consistent with the yields of core-collapse supernovae, i.e. progenitor stars with $20 - 40 M_{\odot}$

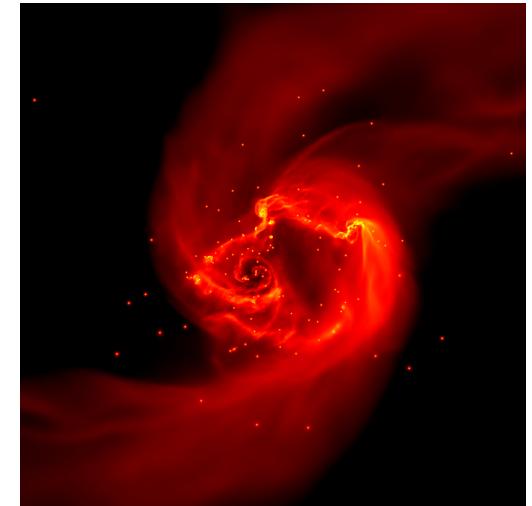
(e.g. Tominaga et al. 2007, Izutani et al. 2009, Joggerst et al. 2009, 2010)

primordial star formation

- just like in present-day SF, we expect

- *turbulence*
 - *thermodynamics (i.e. heating vs. cooling)*
 - *feedback*
 - *magnetic fields*

to influence first star formation.



- masses of first stars still *uncertain*, but we expect a *wide mass range* with *typical masses of several 10s of M_{\odot}*
- disks unstable: first stars in *binaries* or *part of small clusters*
- current frontier: include *feedback* and *magnetic fields* and possibly *dark matter annihilation...*

reducing fragmentation

- from present-day star formation theory we know, that
 - magnetic fields: Peters et al. 2011, Seifried et al. 2012, Hennebelle et al. 2011
 - accretion heating: Peters et al. 2010, Krumholz et al. 2009, Kuipers et al. 2011can influence the fragmentation behavior.
- in the context of Pop III
 - radiation: Hosokawa et al. 2012, Stacy et al. 2012a
 - magnetic fields: Turk et al. 2012, but see also Bovino et al. 2013
Schleicher et al. 2010, Sur et al. 2010, Federrath et al. 2011, Schober et al. 2012ab, 2013
- all these will reduce degree of fragmentation
(but not by much, see Rowan Smith et al. 2011, 2012, at least for accretion heating)
- DM annihilation might become important for disk dynamics and fragmentation (Ripamonti et al. 2011, Stacy et al. 2012b, Rowan Smith et al. 2012)



Carina with HST

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



Carina with HST

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

- stars form from the
of competing processes (such as
pressure)
- **thermodynamic properties**
in the star formation process
- detailed studies require the
physical processes
- star formation is
poorly understood
- **primordial star formation**
star formation

research agenda for the coming years

- **theoretical**
- it requires a
and
- **technical development**
with
various
- **scientific goal**
*dynamics of the interstellar medium
and star clusters*

research agenda for the coming years

- **questions**

- what regulates star formation on galactic scales? global SF relations?
- what drives interstellar turbulence?
- how do molecular clouds form and evolve?
is there unaccounted (molecular) gas in galaxies?
- what are the initial conditions for star cluster formation?
how does cloud structure translate into cluster structure?
- what processes determine the initial mass function (IMF) of stars?
- how does star formation depend on metallicity? how do the first stars form?
- star formation in extreme environments (galactic center, starburst, etc.), how does it differ from a more “normal” mode?

THANKS

