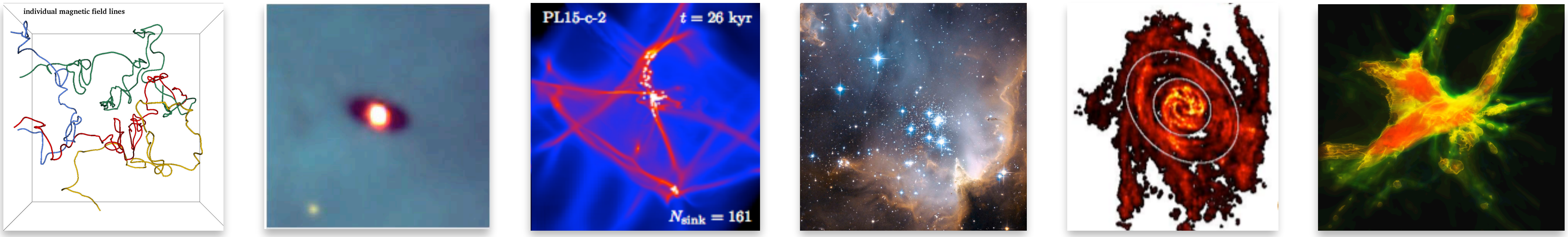
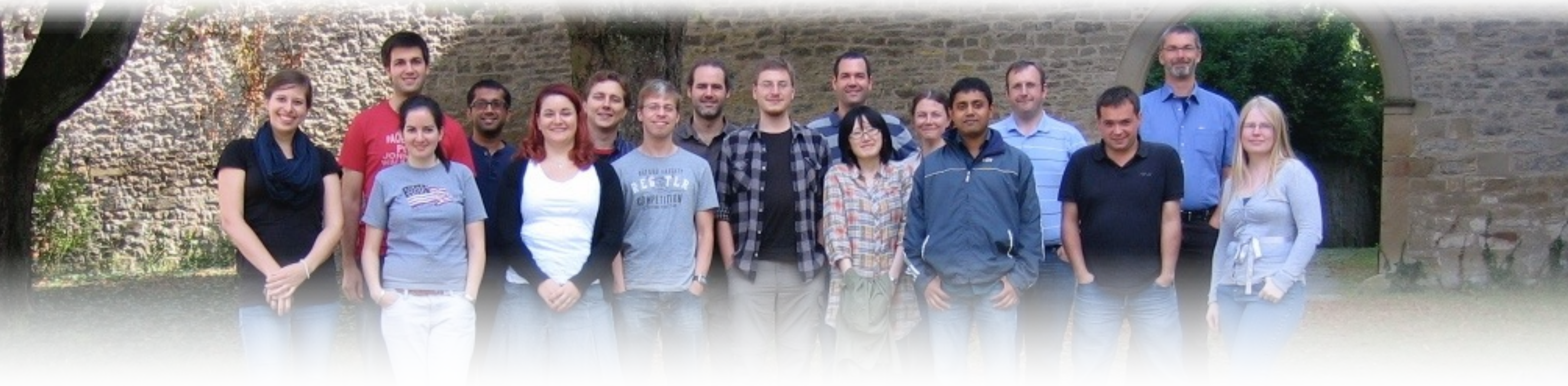
Star Formation



Ralf Klessen

Zentrum für Astronomie der Universität Heidelberg
Institut für Theoretische Astrophysik

thanks to ...



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

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

... 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!

Deutsche Forschungsgemeinschaft DFG
DFG Priority Program 1573 ISM-SPP Interstellar Medium
BADEN-WÜRTTEMBERG STIFTUNG Wir stiften Zukunft
HGSFP
IMPRS
erc European Research Council

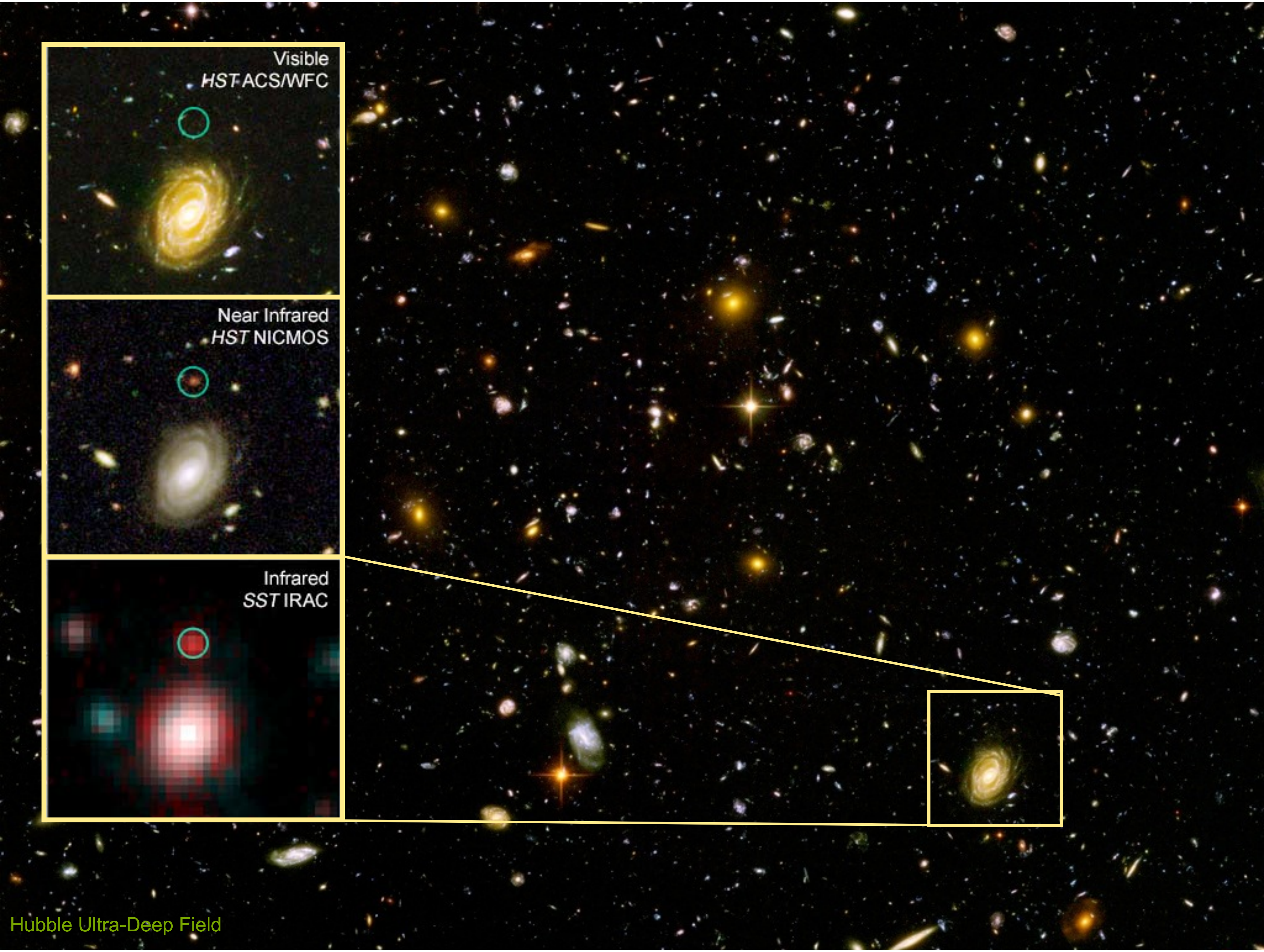
agenda

- 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)

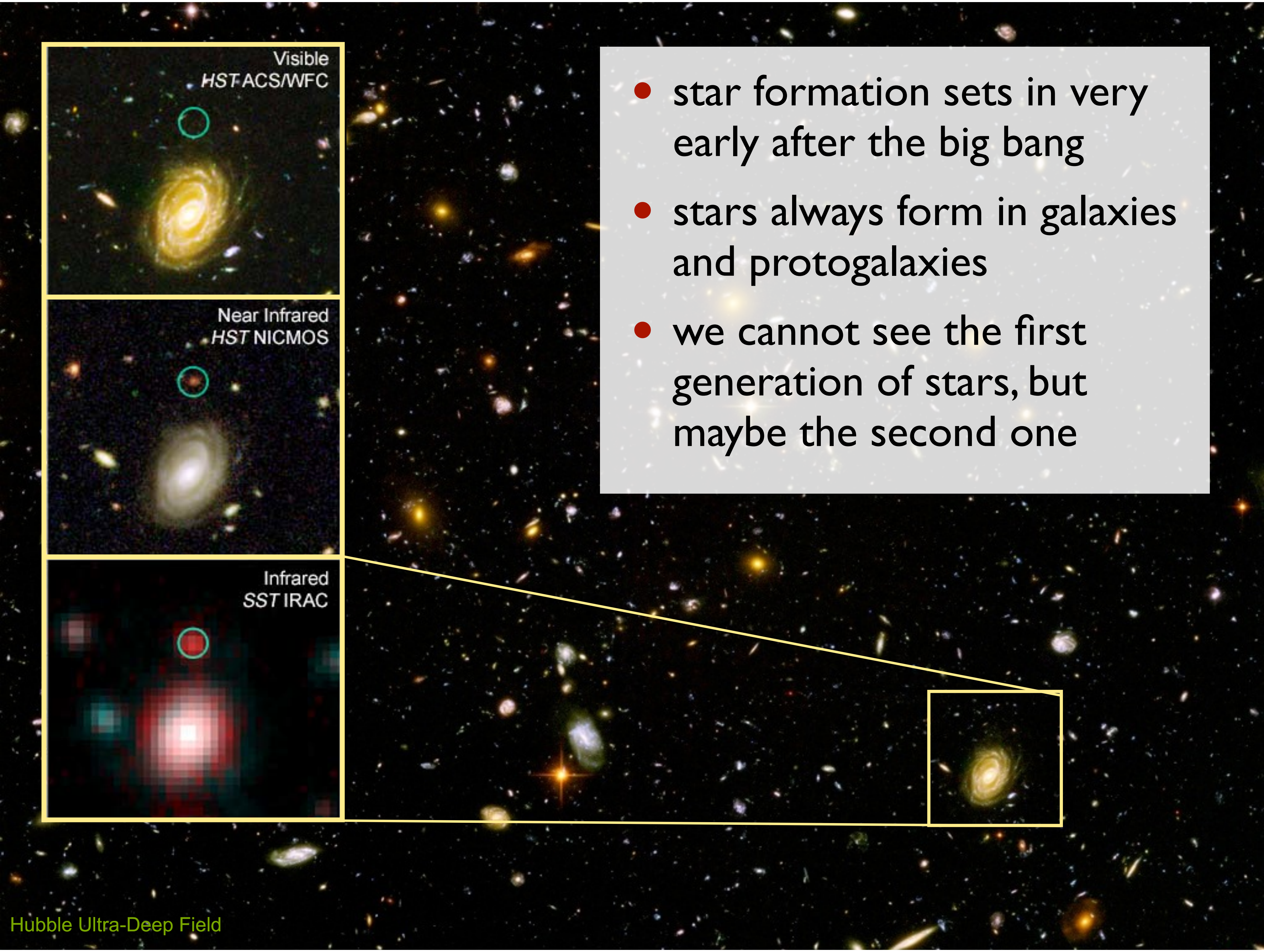
Phenomenology

Hubble Ultra-Deep Field

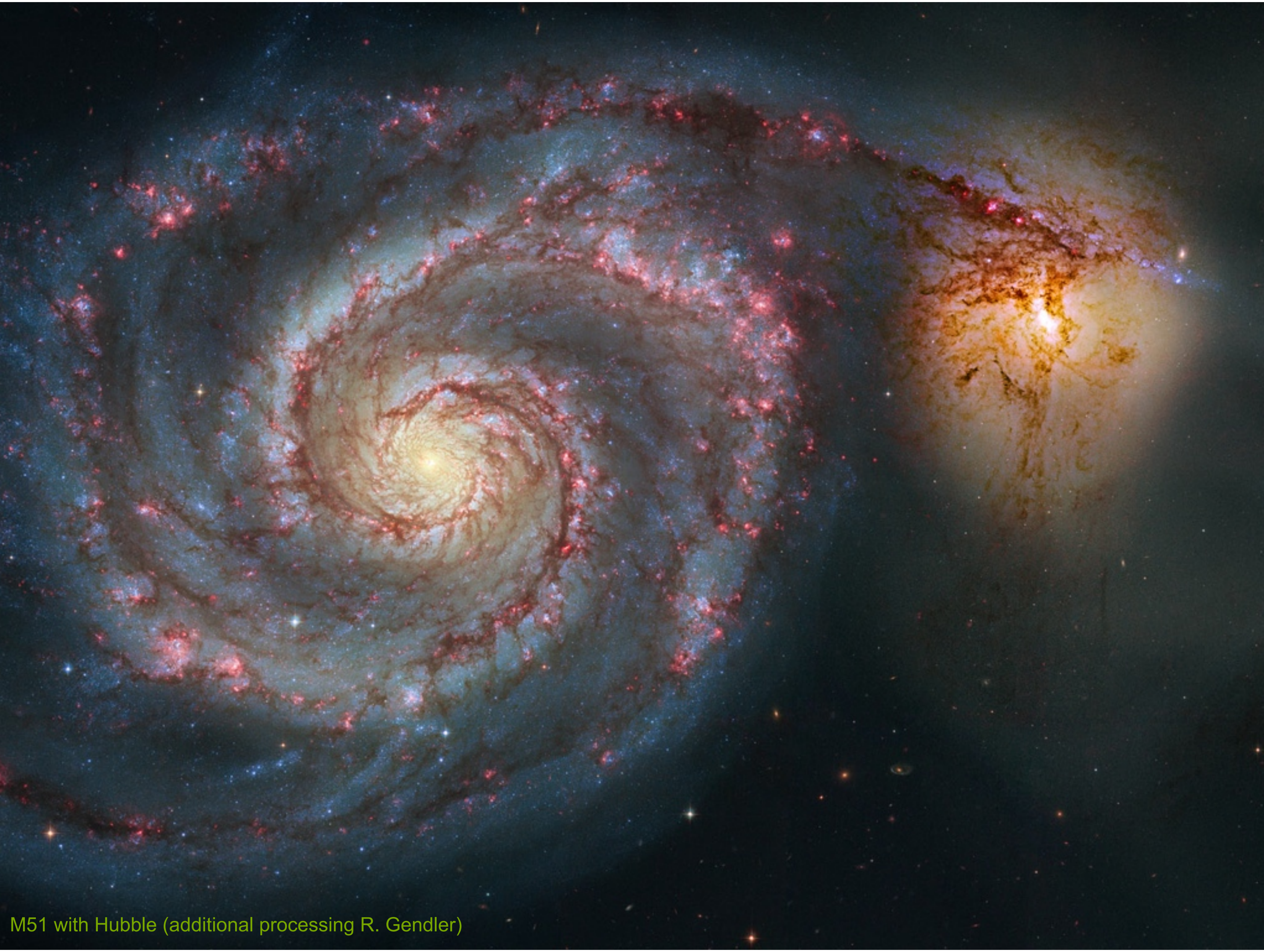


Hubble Ultra-Deep Field

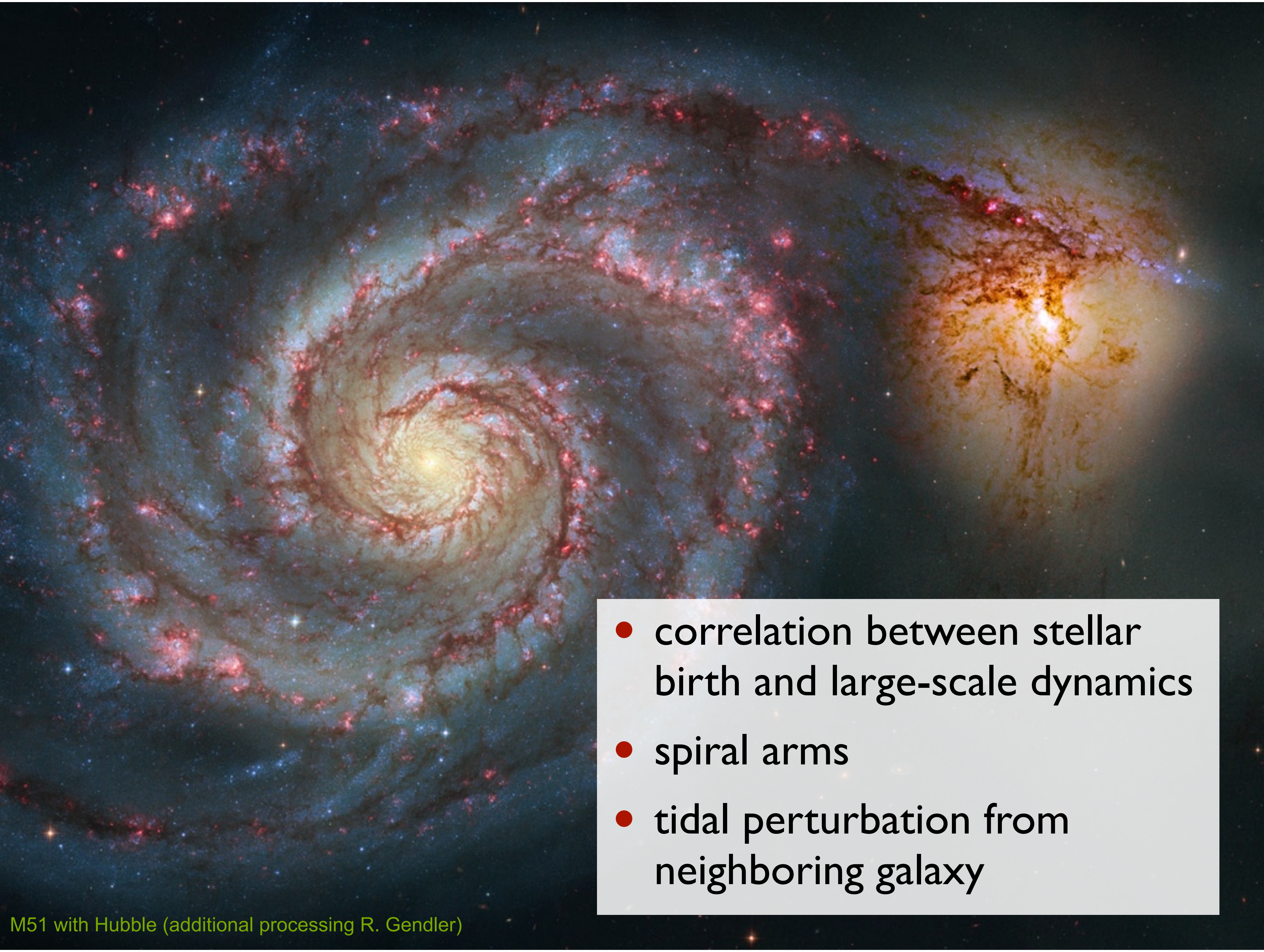
- star formation sets in very early after the big bang
- stars always form in galaxies and protogalaxies
- we cannot see the first generation of stars, but maybe the second one



Hubble Ultra-Deep Field

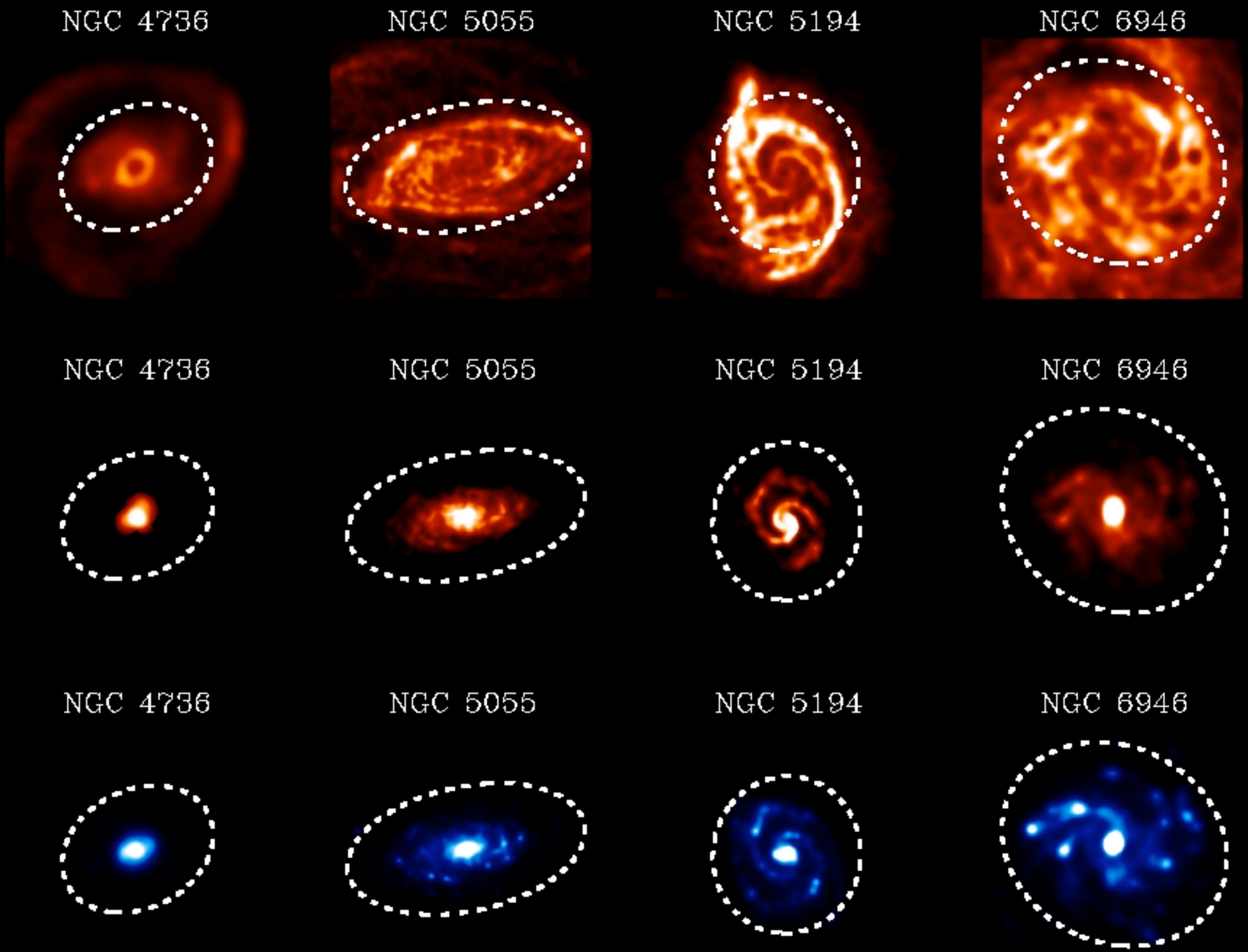


M51 with Hubble (additional processing R. Gendler)



M51 with Hubble (additional processing R. Gendler)

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

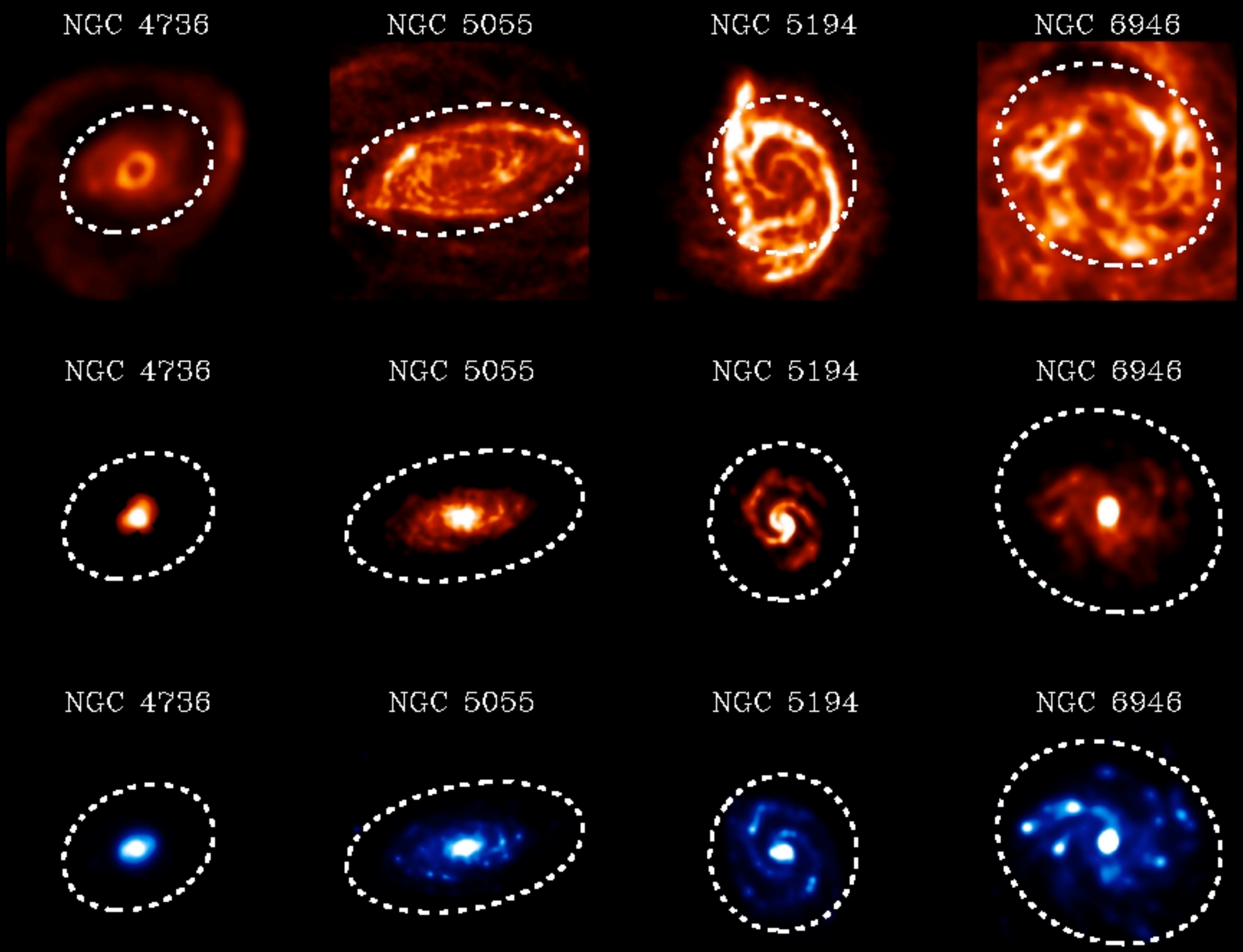


atomic hydrogen

molecular hydrogen

star formation

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



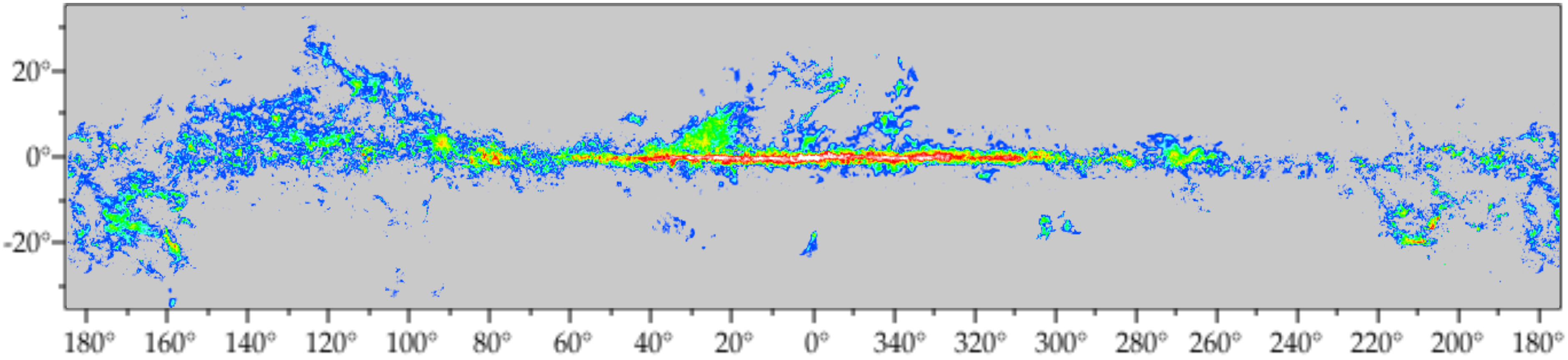
atomic hydrogen

molecular hydrogen

star formation

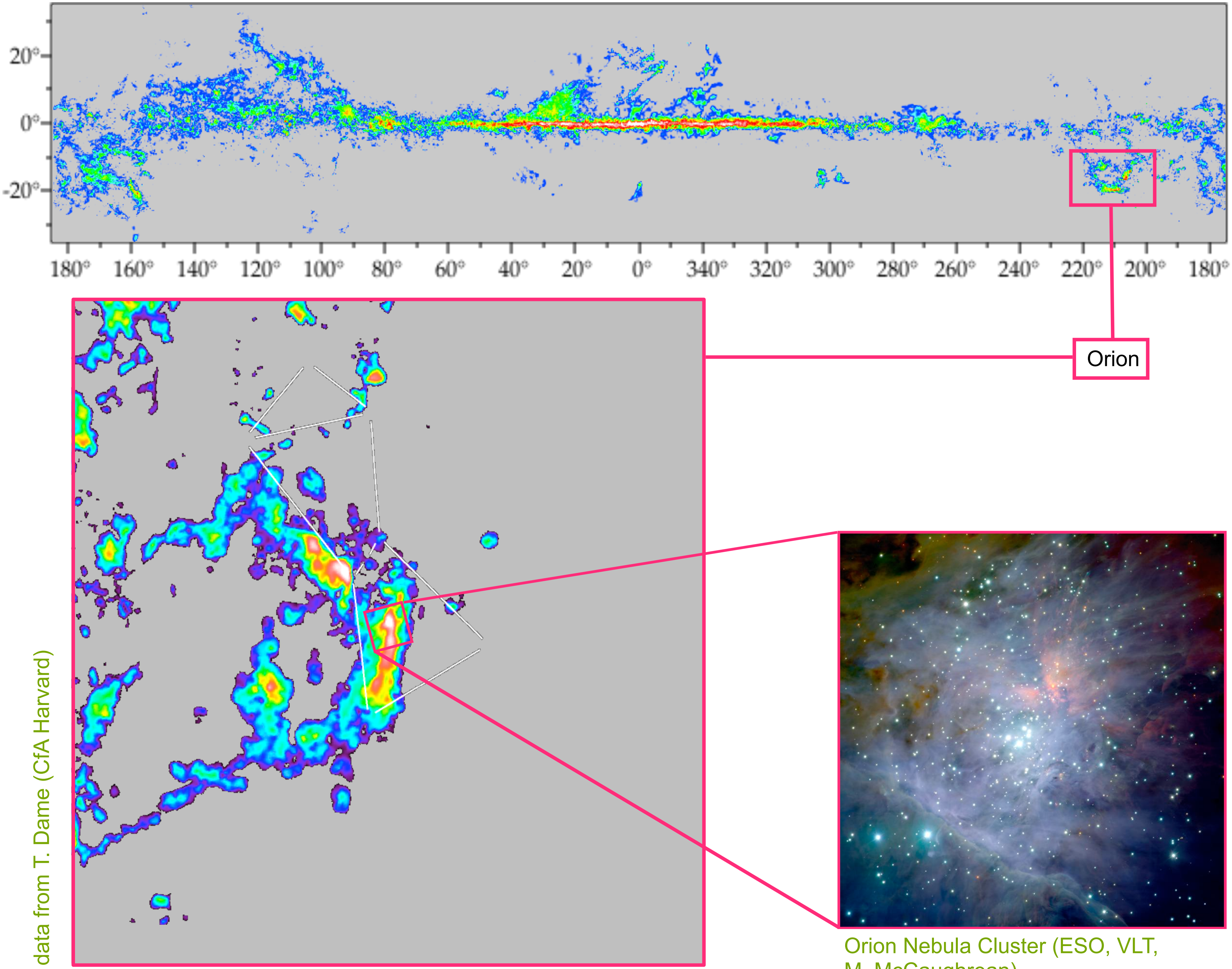
- HI gas more extended
- H2 and SF well correlated

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



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

data from T. Dame (CfA Harvard)



data from T. Dame (CfA Harvard)

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

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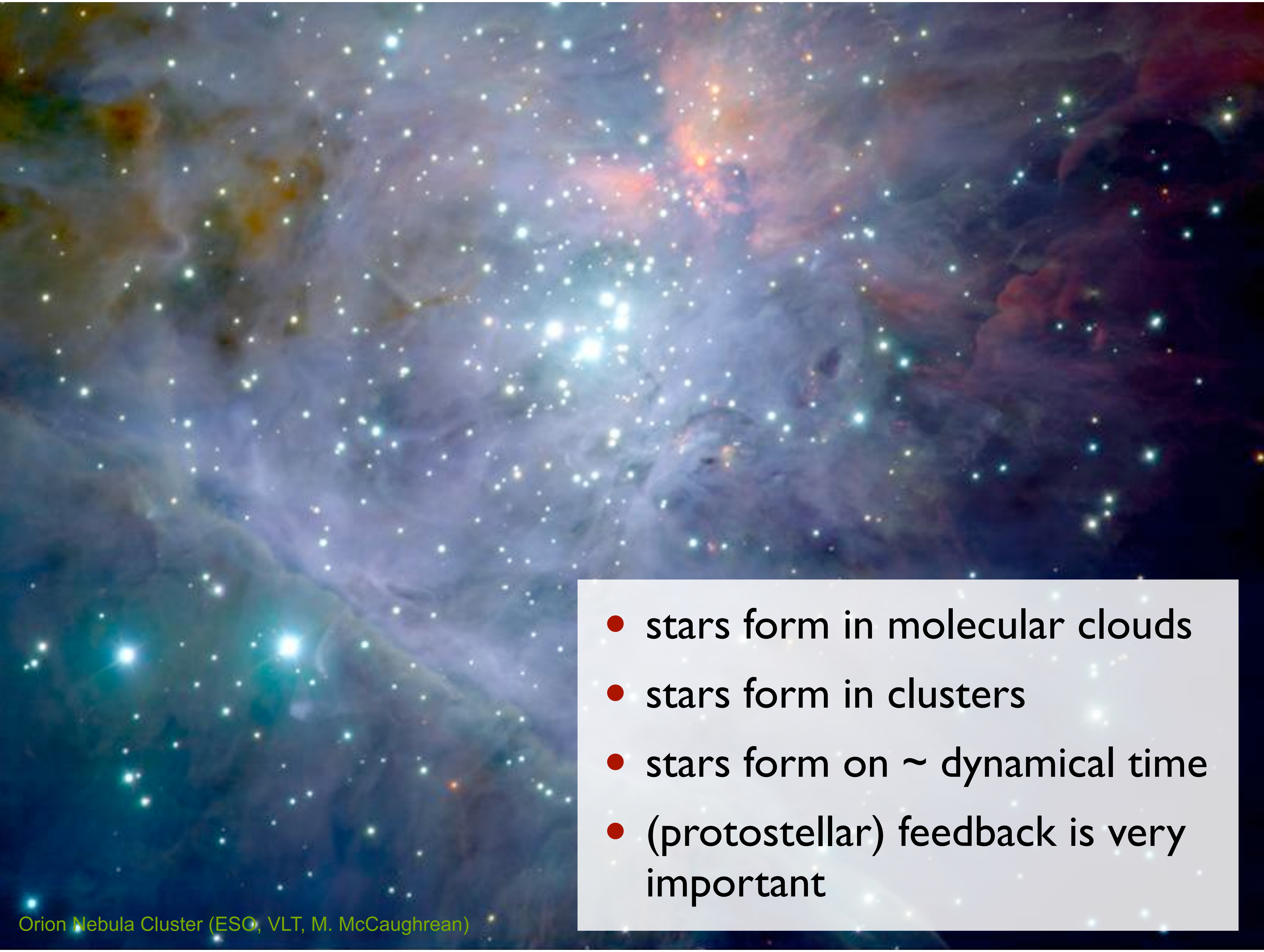
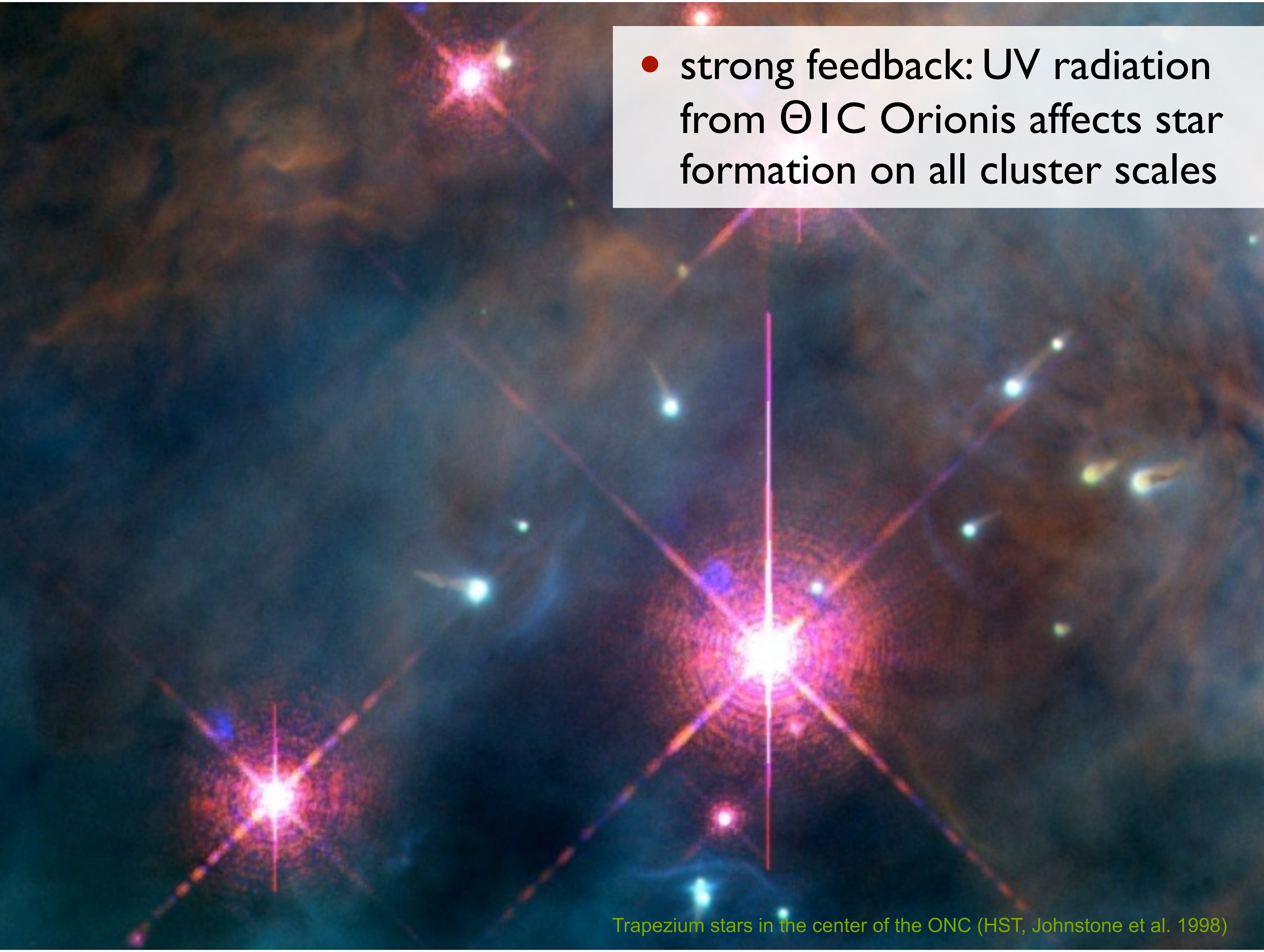


Orion Nebula Cluster (ESO, VLT, M. McCaughrean)

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

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)

Pleiades (DSS, Palomar Observatory Sky Survey)

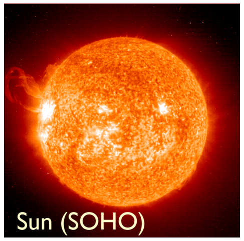
theoretical approach

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: ~ 1 pc
  - size of Sun: 1.4×10^{10} cm

decrease in spatial scale / increase in density


Andromeda (R. Gendler)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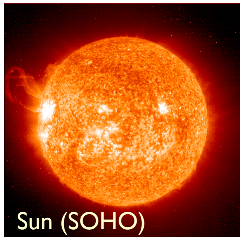
Proplyd in Orion (Hubble)


Sun (SOHO)


Earth

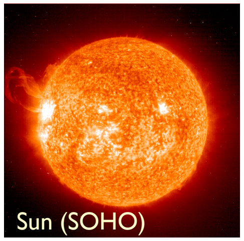
- contracting force
  - only force that can do this compression is *GRAVITY*
- opposing forces
  - there are several processes that can oppose gravity
  - *GAS PRESSURE*
  - *TURBULENCE*
  - *MAGNETIC FIELDS*
  - *RADIATION PRESSURE*

decrease in spatial scale / increase in density


Andromeda (R. Gendler)


NGC 602 in LMC (Hubble)


Proplyd in Orion (Hubble)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  - *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

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

  - instability when $\omega^2 < 0$
  - minimal mass: $\boxed{M_J = \frac{1}{6}\pi^{-5/2} G^{-3/2} \rho_0^{-1/2} c_s^3 \propto \rho_0^{-1/2} T^{+3/2}}$

first approach to turbulence

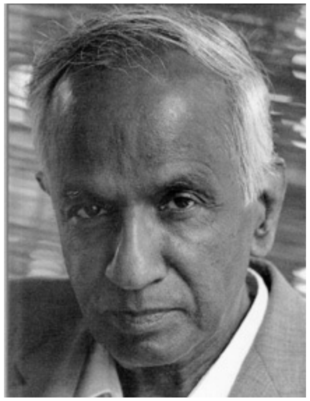
- *von Weizsäcker (1943, 1951)* and *Chandrasekhar (1951):* concept of ***MICROTURBULENCE***
  - BASIC ASSUMPTION: separation of scales between dynamics and turbulence

    $\ell_{\rm turb} \ll \ell_{\rm dyn}$
  - then turbulent velocity dispersion contributes to effective soundspeed:

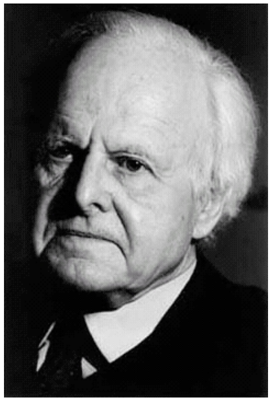
$$\boxed{c_c^2 \mapsto c_c^2 + \sigma_{rms}^2}$$

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

    (2) supersonic turbulence → $\sigma_{rms}^2(k) >> c_s^2$ *usually*



S. Chandrasekhar, 1910 - 1995



C.F. von Weiszäcker, 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 *~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

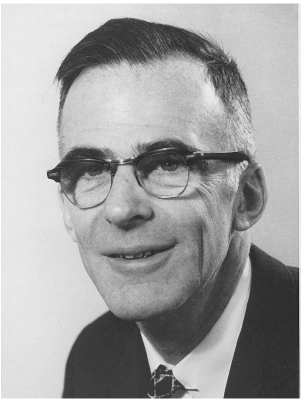
- *Mestel & Spitzer (1956):* Magnetic fields can prevent collapse*!!!*
  - Critical mass for gravitational collapse in presence of B-field

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

  - 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

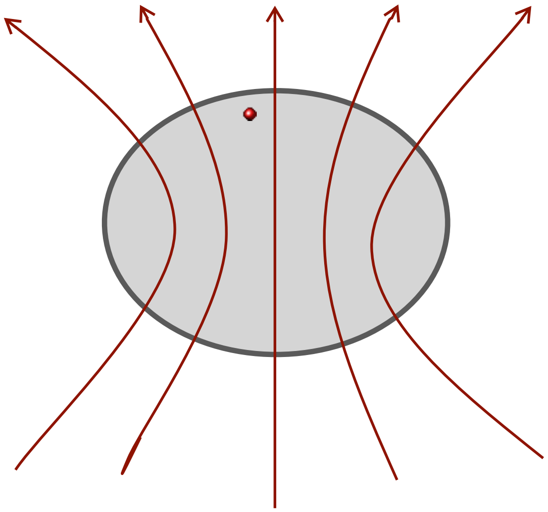


Lyman Spitzer, Jr., 1914 - 1997

“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 ($\tau_{ff} << \tau_{AD}$) (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)

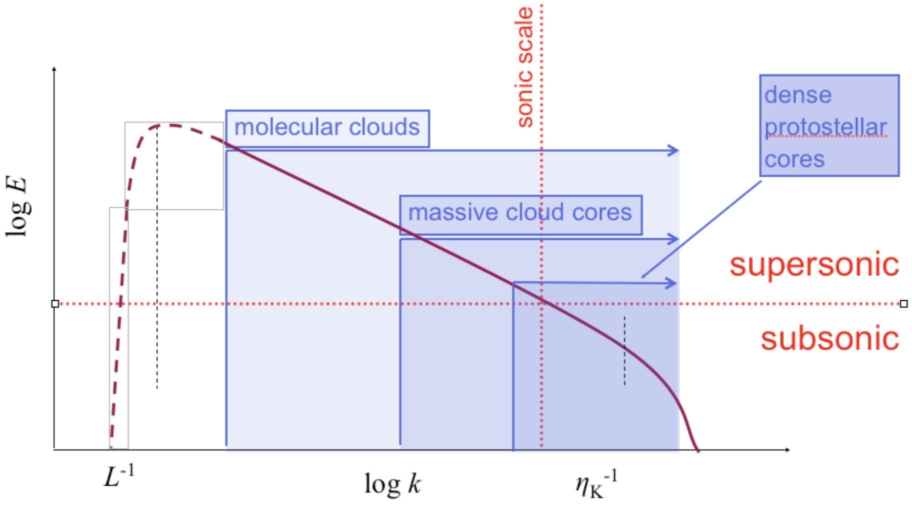
(see e.g. Mac Low & Klessen, 2004, Rev. Mod. Phys., 76, 125-194)

gravoturbulent star formation

- BASIC ASSUMPTION:

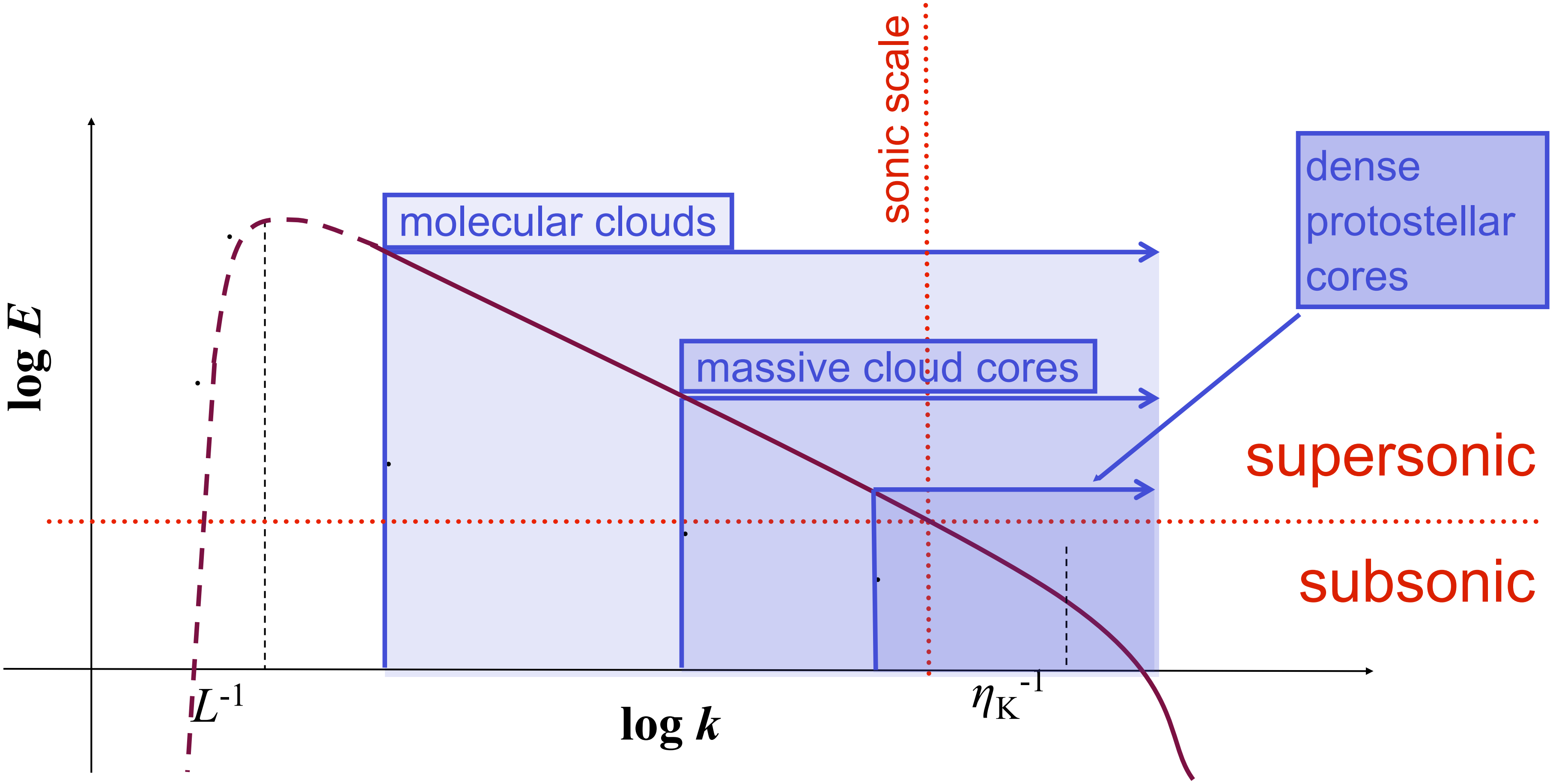
star formation is controlled by interplay between supersonic turbulence and self-gravity

- 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 . . .



Mac Low & Klessen, 2004, Rev. Mod. Phys., 76, 125-194
McKee & Ostriker, 2007, ARAA, 45, 565

turbulent cascade in the ISM



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

$\sigma_{rms} << 1$ km/s

$M_{rms} \leq 1$

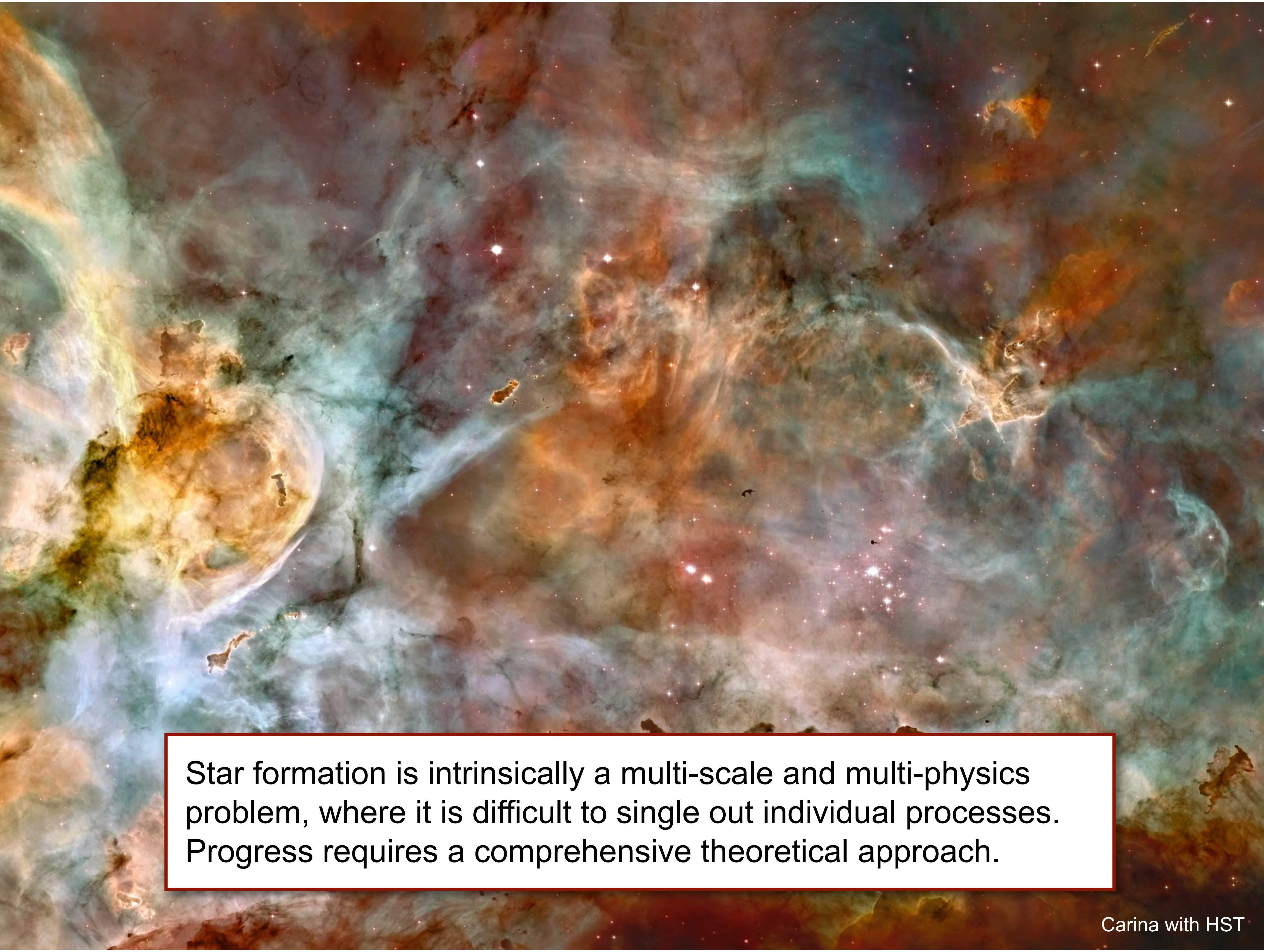
$L \approx 0.1$ pc

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

current status

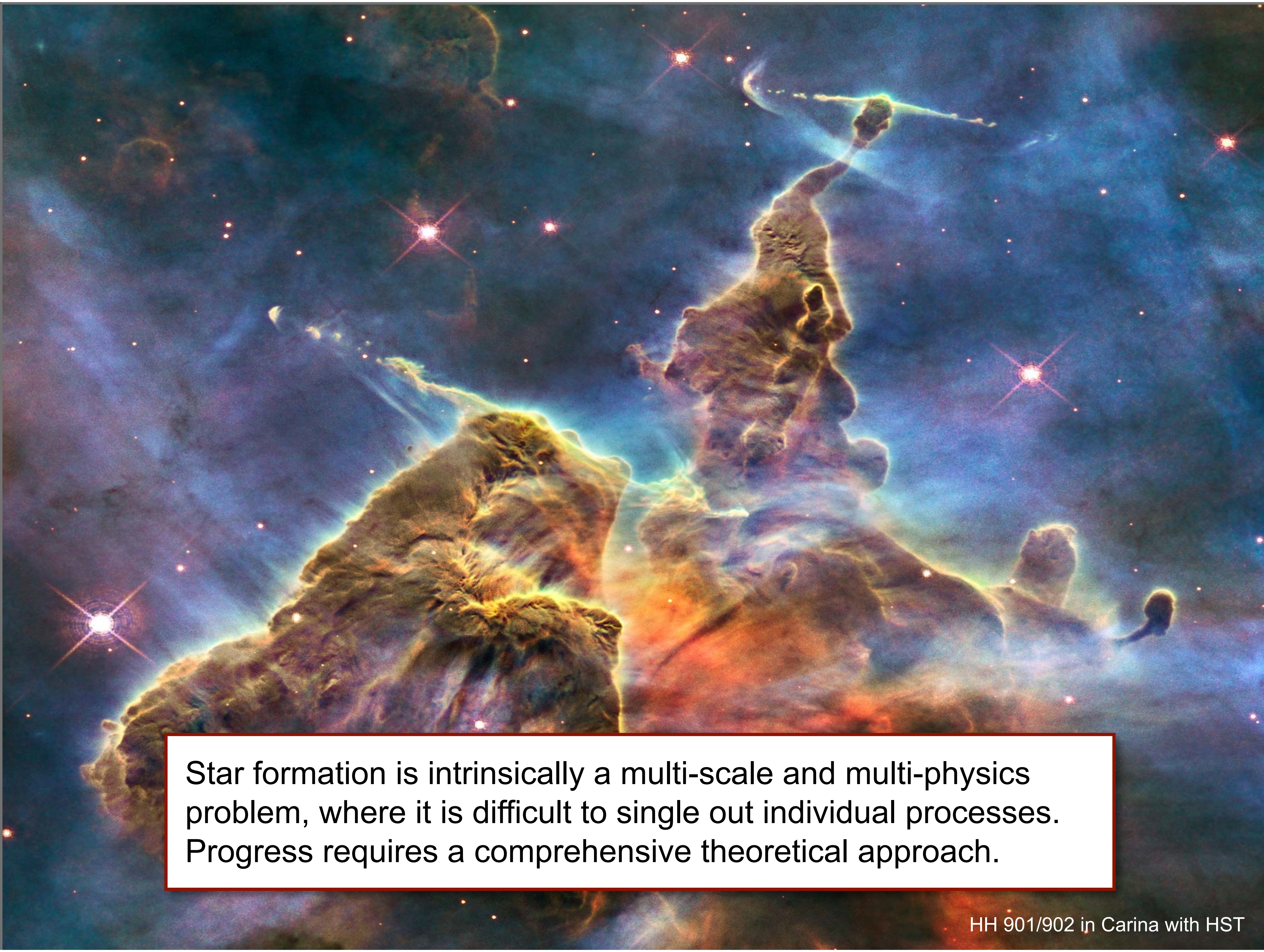
- *stars form from the complex interplay of self-gravity and a large number of competing processes (such as turbulence, magnetic fields, radiative and mechanical feedback, thermal pressure, cosmic rays, etc.)*
- *the relative importance of these processes depends on the environment*
  - prestellar cores --> thermal pressure is important
molecular clouds --> turbulence dominates } (Larson's relation: $\sigma \propto L^{1/2}$)
  - 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.



Star formation is intrinsically a multi-scale and multi-physics problem, where it is difficult to single out individual processes. Progress requires a comprehensive theoretical approach.

Carina with HST

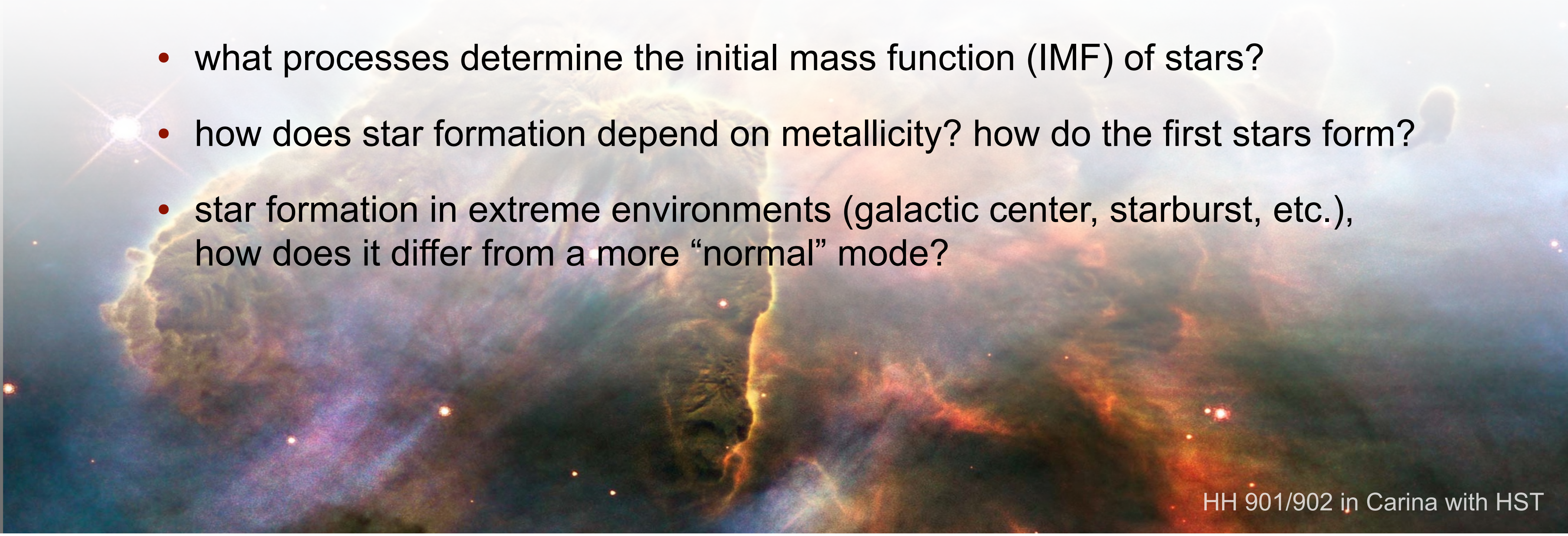


Star formation is intrinsically a multi-scale and multi-physics problem, where it is difficult to single out individual processes. Progress requires a comprehensive theoretical approach.

HH 901/902 in Carina with HST

selected open questions

- what regulates star formation on galactic scales? global SF relations?
- what drives interstellar turbulence 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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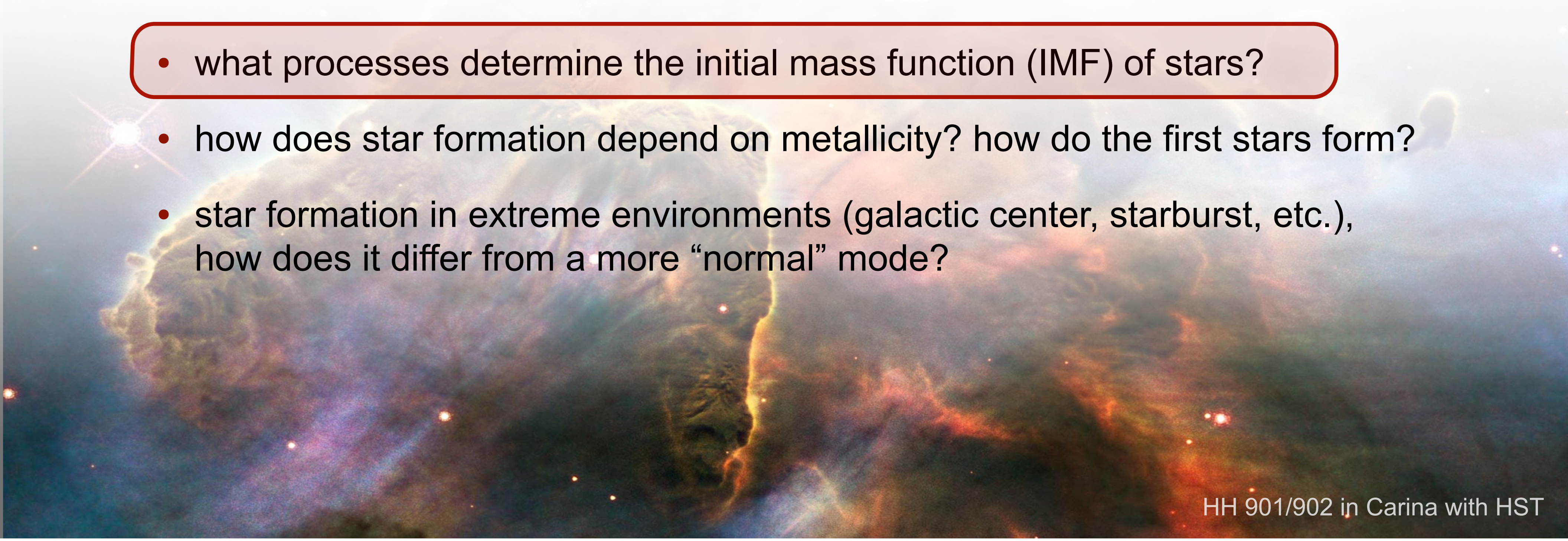
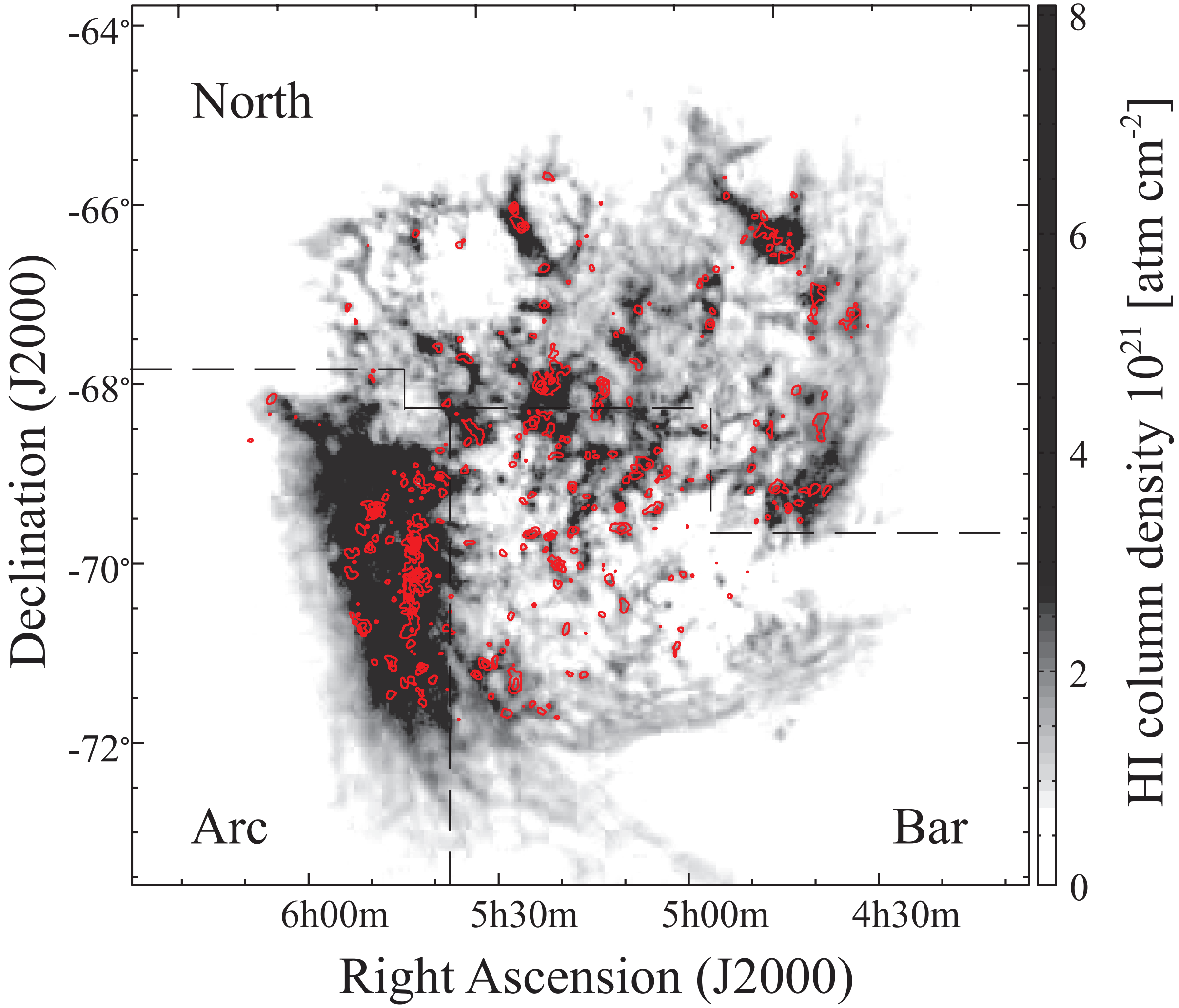


HH 901/902 in Carina with HST

molecular cloud formation

molecular cloud formation



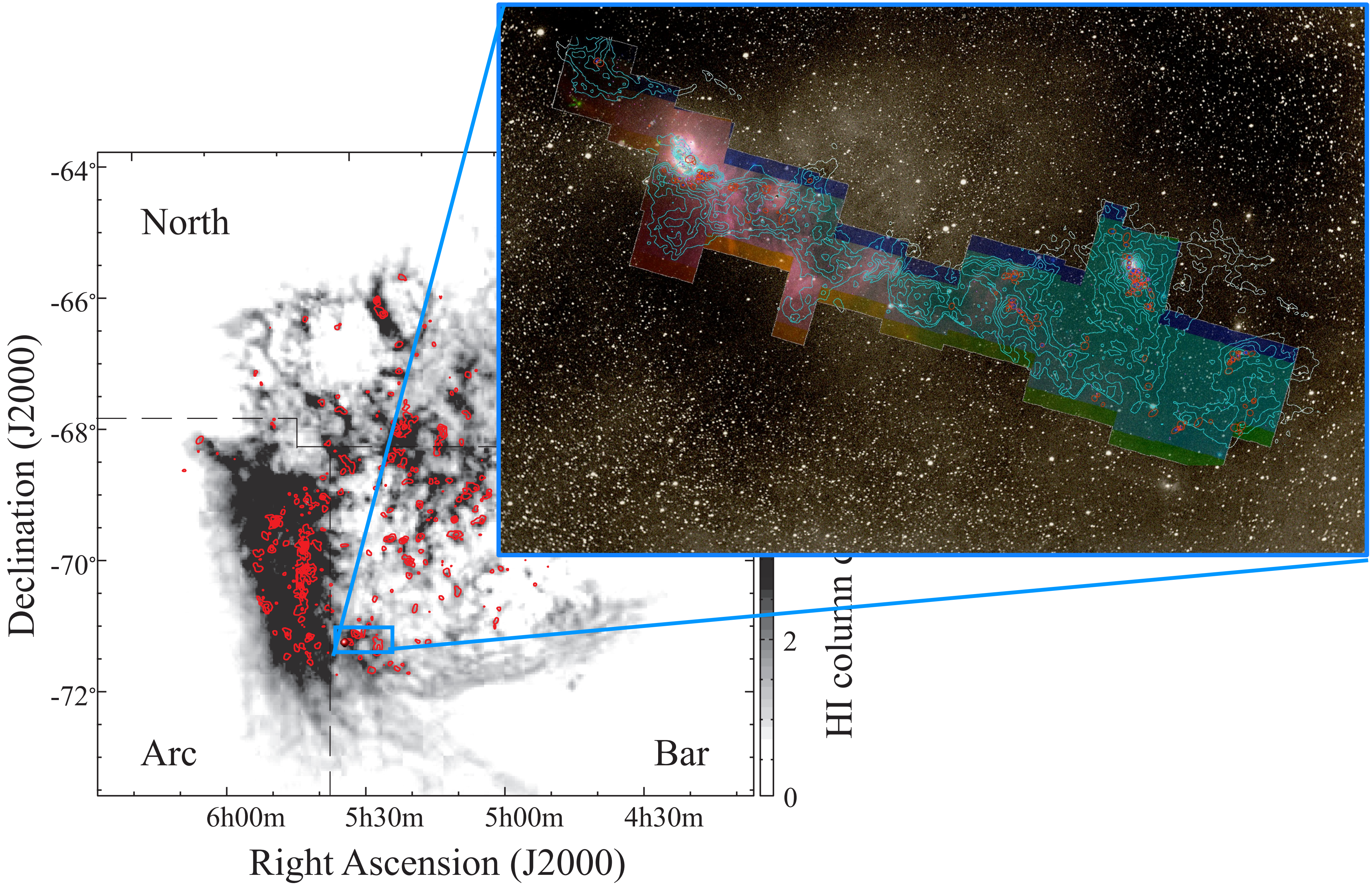
Fukui et al. (2009)

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 ...


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

position-position-velocity structure of the Perseus cloud

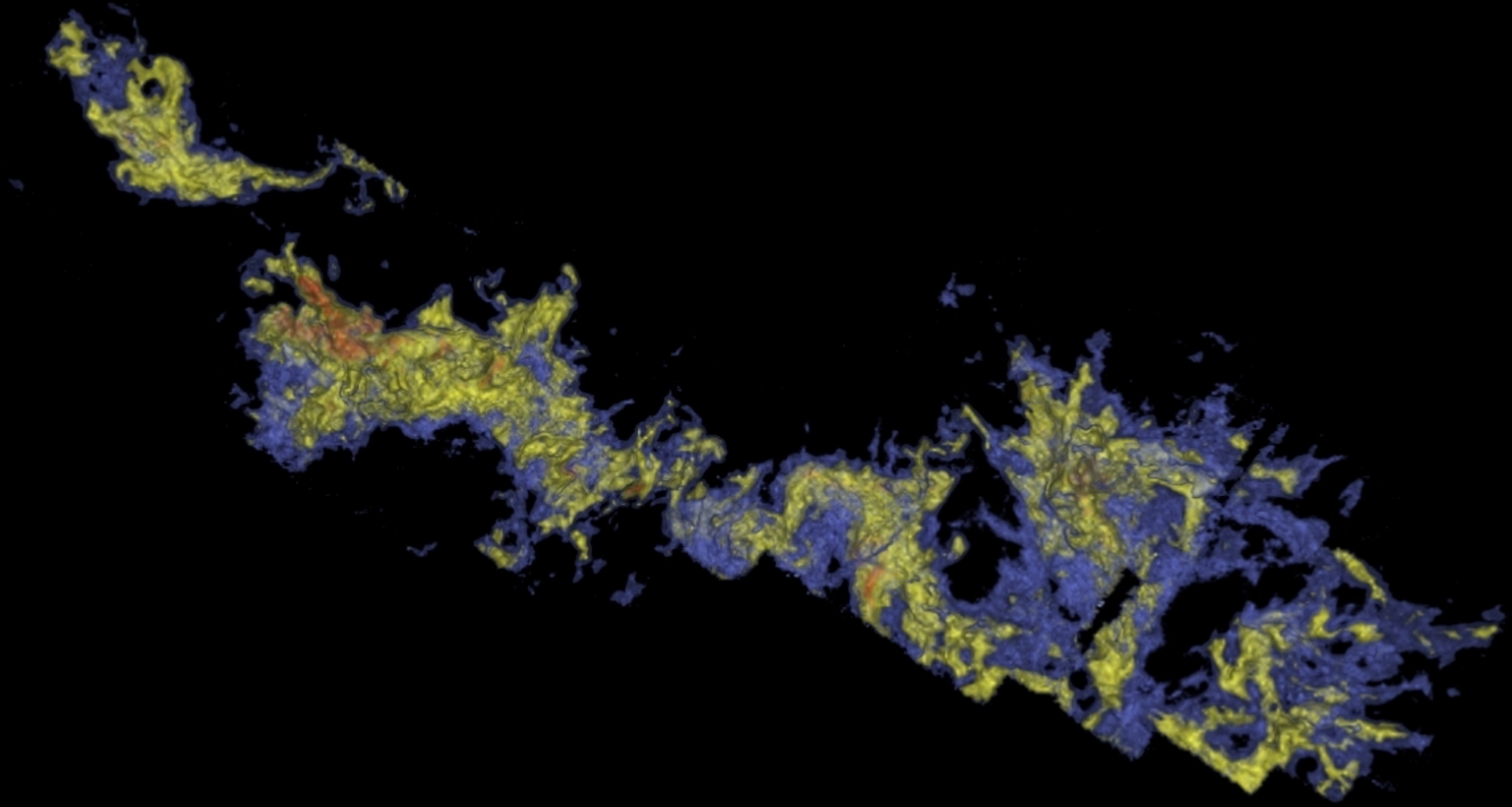
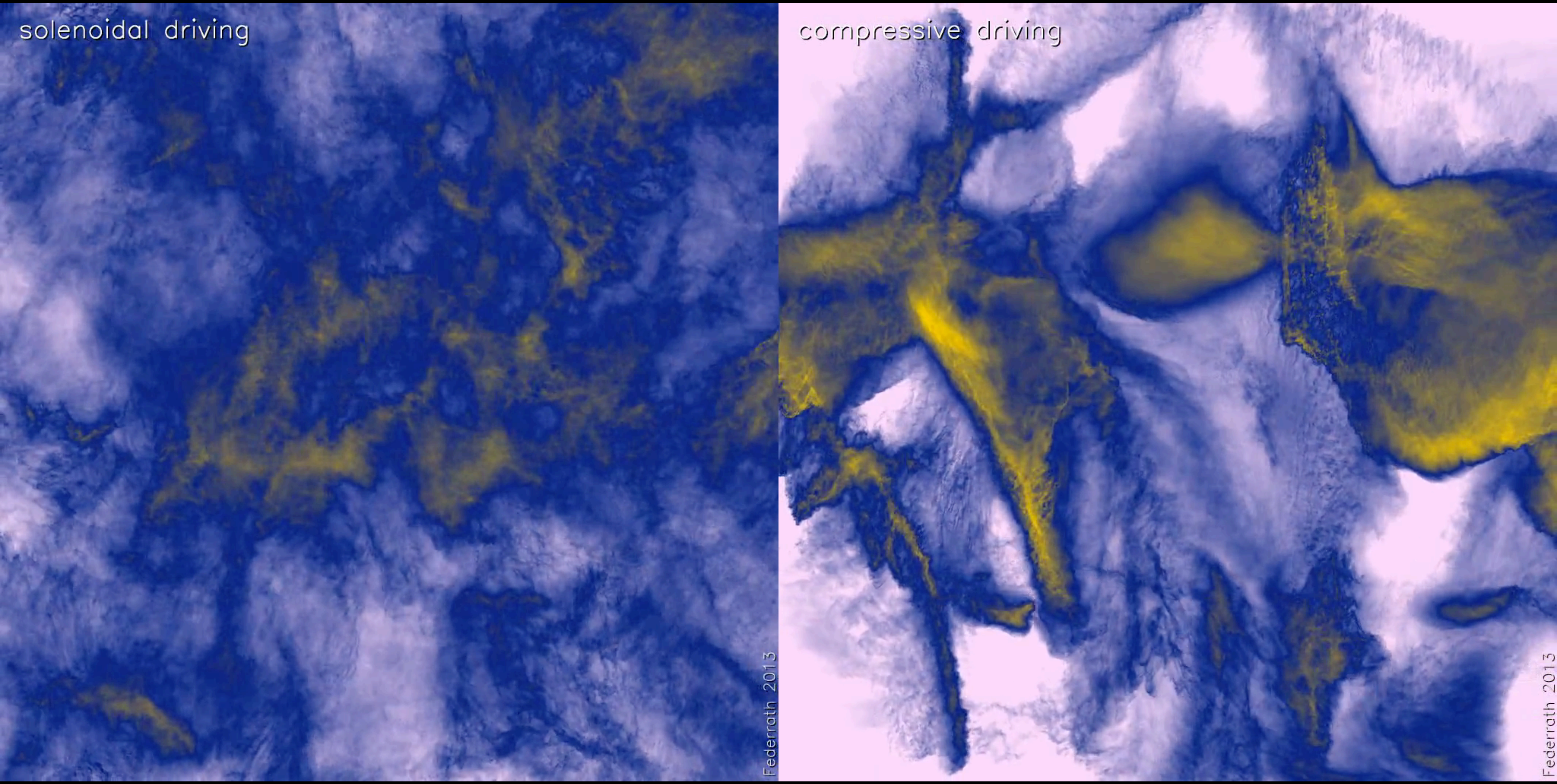


image from Alyssa Goodman: COMPLETE survey

density structure resulting from different turbulent driving schemes



driving with solenoidal modes

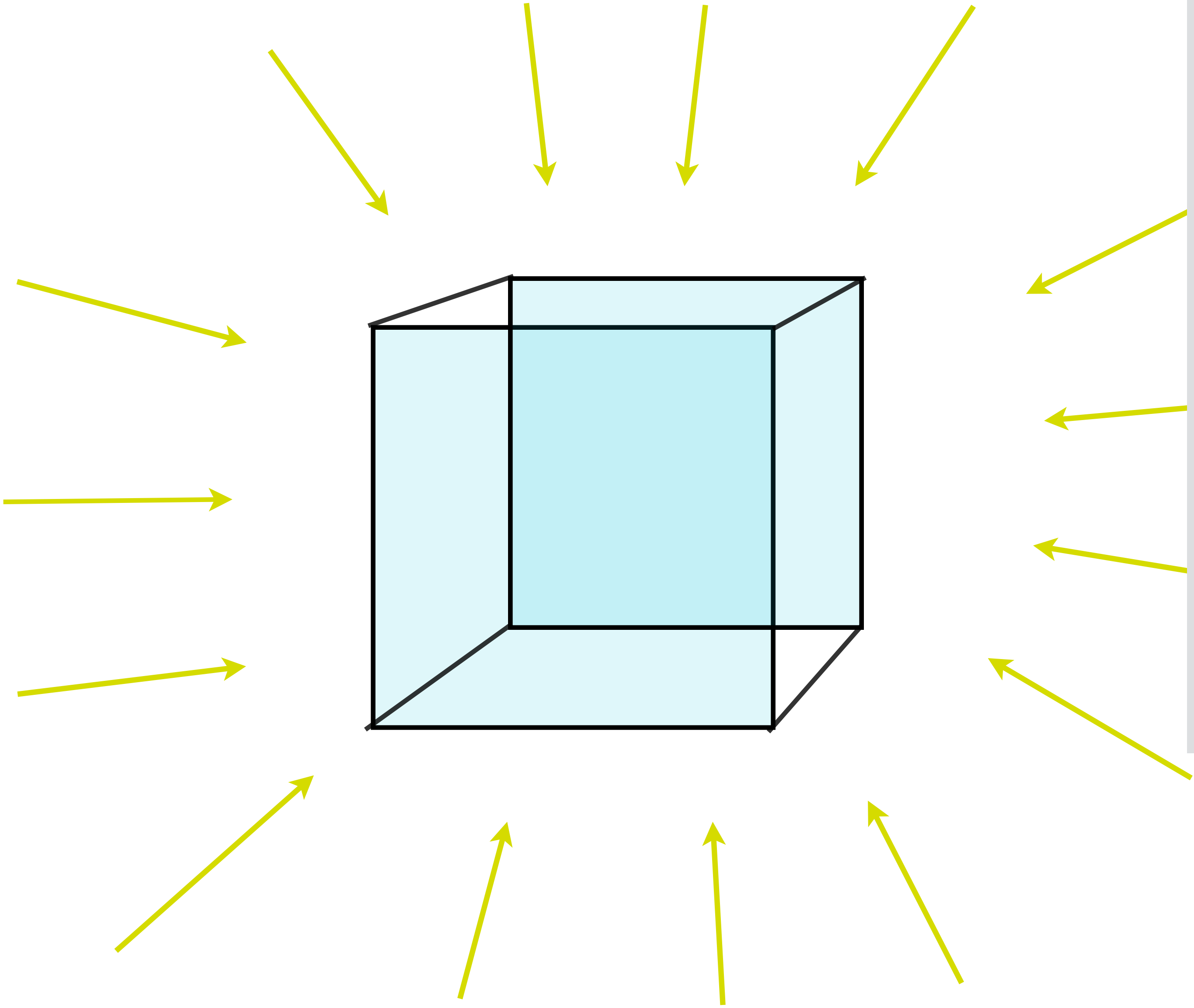
driving with compressive modes

(turbulent box of isothermal ideal gas resolution 4096^3 cells)

Federrath (2013, MNRAS, 436, 1245)

including detailed chemistry

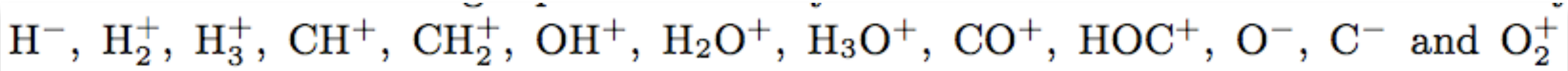
experimental set-up



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

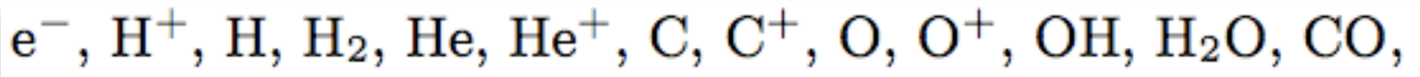
chemical model 0

- 32 chemical species
  - 17 in instantaneous equilibrium:

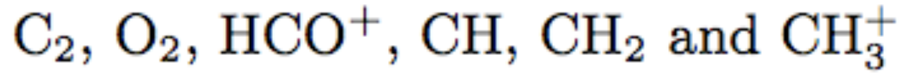


H^-, H_2^+, H_3^+, CH^+, CH_2^+, OH^+, H_2O^+, H_3O^+, CO^+, HOC^+, O^-, C^- and O_2^+

  - 19 full non-equilibrium evolution



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

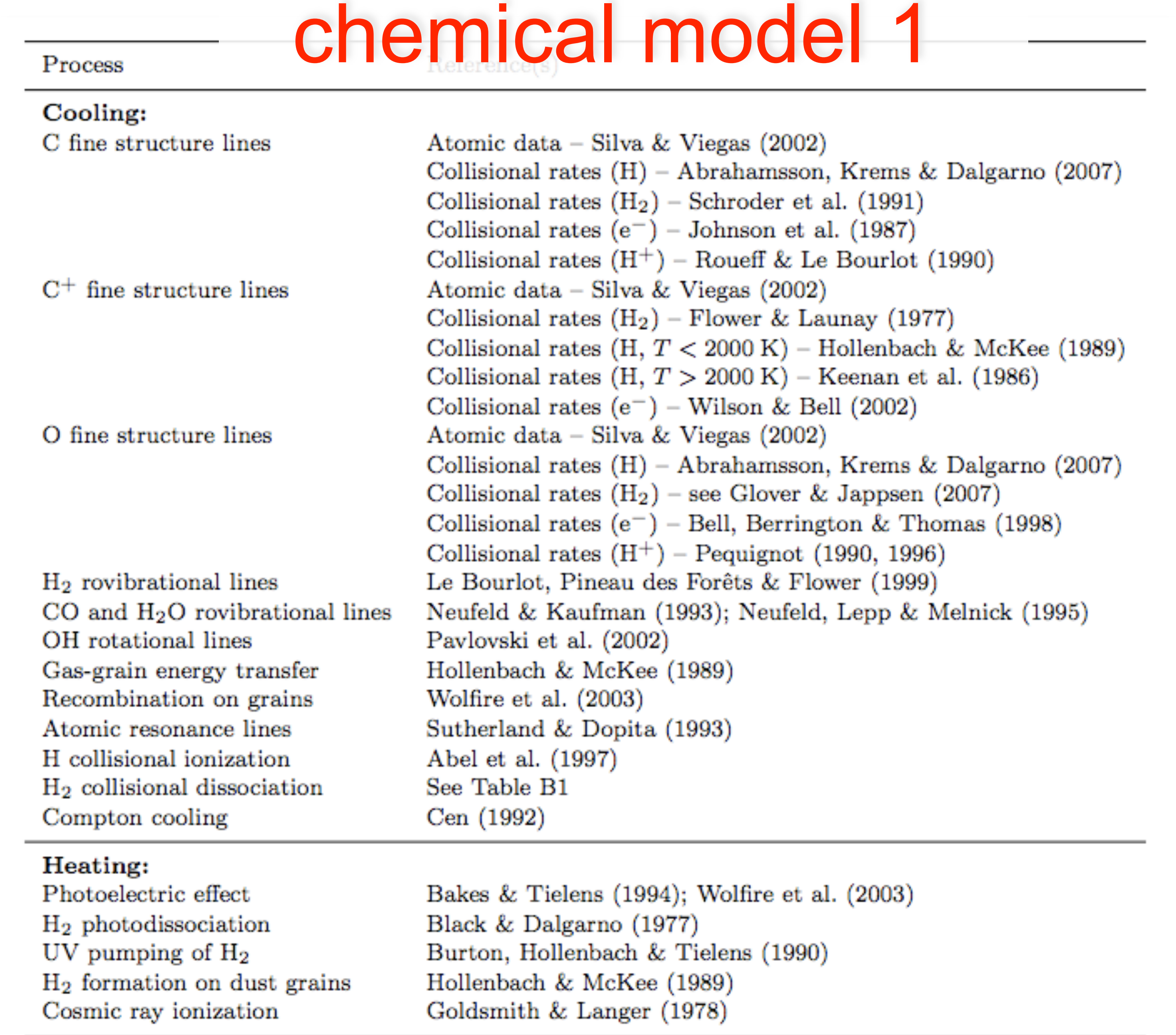


C_2, O_2, HCO^+, CH, CH_2 and CH_3^+

- 218 reactions
- various heating and cooling processes

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

chemical model 1



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

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

chemical model 2

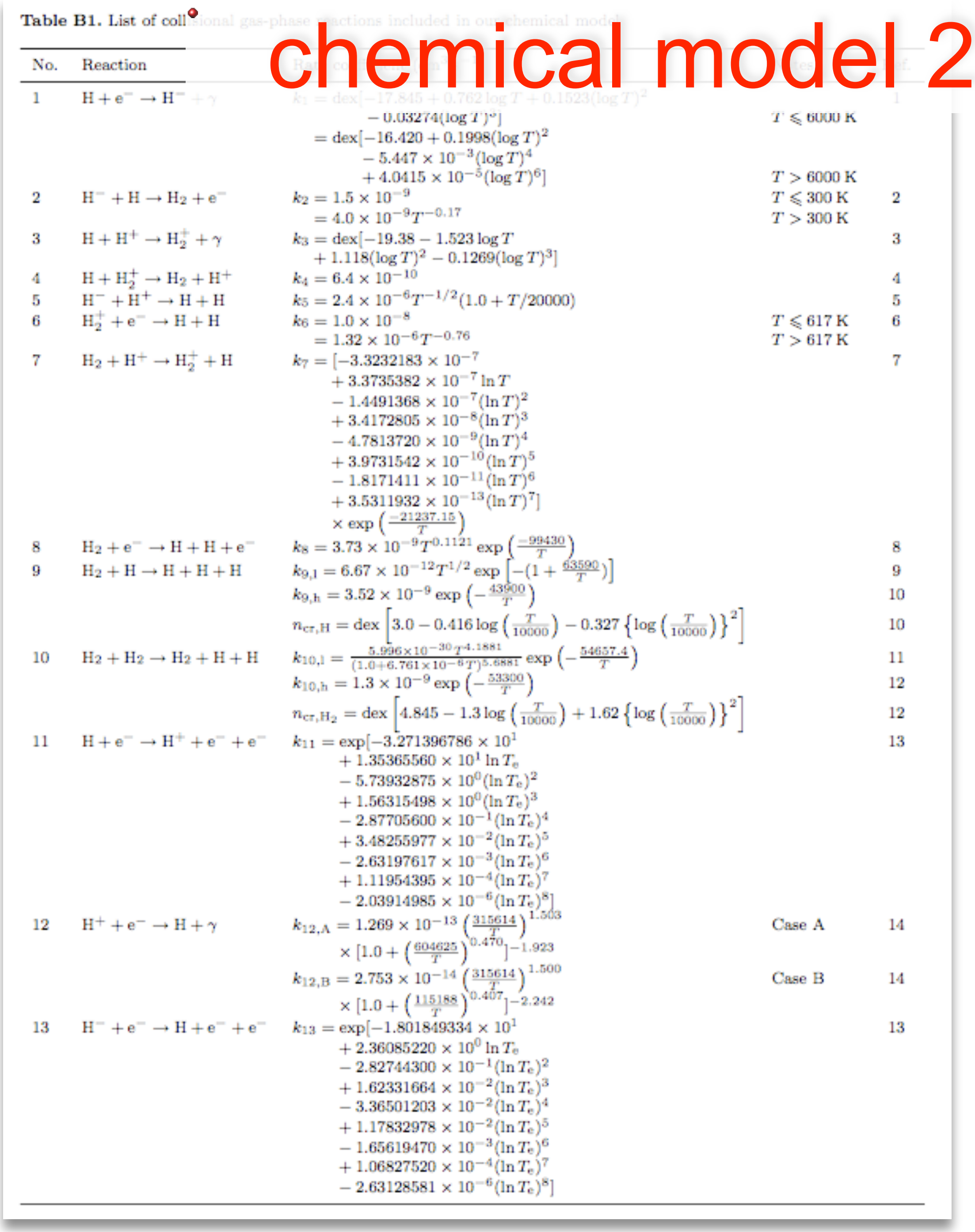


Table B1. List of collisional gas-phase reactions included in our chemical model.

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

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chemical model 2

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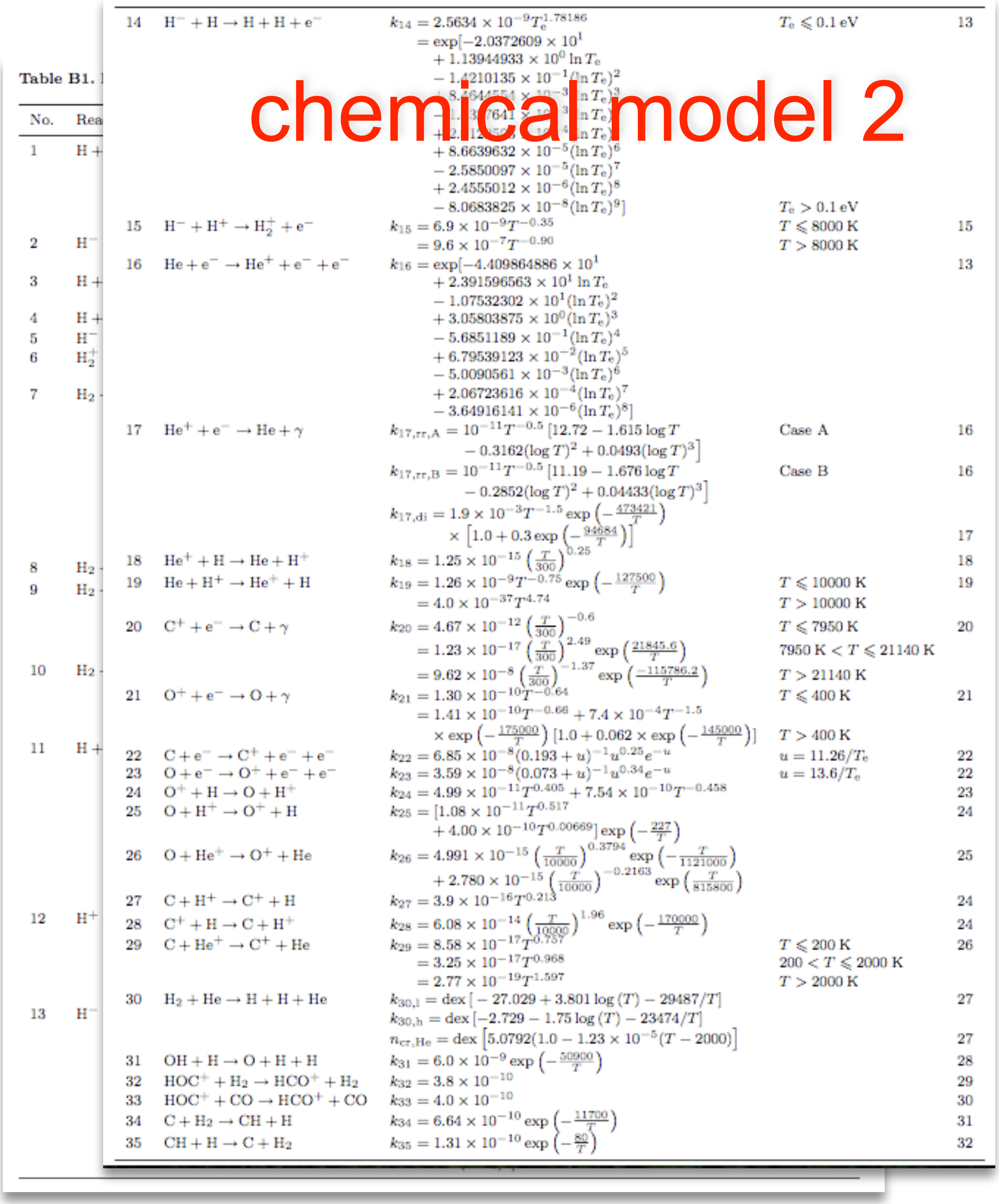


Table B1.

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

14	$H^- + H \rightarrow H + H + e^-$	$k_{14} = 2.5634 \times 10^{-9} T_e^{1.78186}$	$T_e \leqslant 0.1$ eV	13
		$= \exp[-2.0372609 \times 10^{1}$		
		$+ 1.13944933 \times 10^{0} \ln T_e$		
		$- 1.4210135 \times 10^{-1} (\ln T_e)^2$		
		$+ 8.4644554 \times 10^{-3} (\ln T_e)^3$		
		$- 1.4327641 \times 10^{-3} (\ln T_e)^4$		
		$+ 2.0122503 \times 10^{-4} (\ln T_e)^5$		
		$+ 8.6639632 \times 10^{-5} (\ln T_e)^6$		
		$- 2.5850097 \times 10^{-5} (\ln T_e)^7$		
		$+ 2.4555012 \times 10^{-6} (\ln T_e)^8$		
		$- 8.0683825 \times 10^{-8} (\ln T_e)^9]$	$T_e > 0.1$ eV	
15	$H^- + H^+ \rightarrow H_2^+ + e^-$	$k_{15} = 6.9 \times 10^{-9} T^{-0.35}$	$T \leqslant 8000$ K	15
		$= 9.6 \times 10^{-7} T^{-0.90}$	$T > 8000$ K	
16	$He + e^- \rightarrow He^+ + e^- + e^-$	$k_{16} = \exp[-4.409864886 \times 10^{1}$		13
		$+ 2.391596563 \times 10^{1} \ln T_e$		
		$- 1.07532302 \times 10^{1} (\ln T_e)^2$		
		$+ 3.05803875 \times 10^{0} (\ln T_e)^3$		
		$- 5.6851189 \times 10^{-1} (\ln T_e)^4$		
		$+ 6.79539123 \times 10^{-2} (\ln T_e)^5$		
		$- 5.0090561 \times 10^{-3} (\ln T_e)^6$		
		$+ 2.06723616 \times 10^{-4} (\ln T_e)^7$		
		$- 3.64916141 \times 10^{-6} (\ln T_e)^8]$		
17	$He^+ + e^- \rightarrow He + \gamma$	$k_{17,rr,A} = 10^{-11} T^{-0.5} [12.72 - 1.615 \log T$	Case A	16
		$- 0.3162 (\log T)^2 + 0.0493 (\log T)^3]$		
		$k_{17,rr,B} = 10^{-11} T^{-0.5} [11.19 - 1.676 \log T$	Case B	16
		$- 0.2852 (\log T)^2 + 0.04433 (\log T)^3]$		
		$k_{17,di} = 1.9 \times 10^{-3} T^{-1.5} \exp\left(-\frac{473421}{T}\right)$		
		$\times \left[1.0 + 0.3 \exp\left(-\frac{94684}{T}\right)\right]$		17
18	$He^+ + H \rightarrow He + H^+$	$k_{18} = 1.25 \times 10^{-15} \left(\frac{T}{300}\right)^{0.25}$		18
19	$He + H^+ \rightarrow He^+ + H$	$k_{19} = 1.26 \times 10^{-9} T^{-0.75} \exp\left(-\frac{127500}{T}\right)$	$T \leqslant 10000$ K	19
		$= 4.0 \times 10^{-37} T^{4.74}$	$T > 10000$ K	
20	$C^+ + e^- \rightarrow C + \gamma$	$k_{20} = 4.67 \times 10^{-12} \left(\frac{T}{300}\right)^{-0.6}$	$T \leqslant 7950$ K	20
		$= 1.23 \times 10^{-17} \left(\frac{T}{300}\right)^{2.49} \exp\left(\frac{21845.6}{T}\right)$	$7950 \text{ K} < T \leqslant 21140$ K	
		$= 9.62 \times 10^{-8} \left(\frac{T}{300}\right)^{-1.37} \exp\left(\frac{-115786.2}{T}\right)$	$T > 21140$ K	
21	$O^+ + e^- \rightarrow O + \gamma$	$k_{21} = 1.30 \times 10^{-10} T^{-0.64}$	$T \leqslant 400$ K	21
		$= 1.41 \times 10^{-10} T^{-0.66} + 7.4 \times 10^{-4} T^{-1.5}$		
		$\times \exp\left(-\frac{175000}{T}\right) [1.0 + 0.062 \times \exp\left(-\frac{145000}{T}\right)]$	$T > 400$ K	
22	$C + e^- \rightarrow C^+ + e^- + e^-$	$k_{22} = 6.85 \times 10^{-8} (0.193 + u)^{-1} u^{0.25} e^{-u}$	$u = 11.26/T_e$	22
23	$O + e^- \rightarrow O^+ + e^- + e^-$	$k_{23} = 3.59 \times 10^{-8} (0.073 + u)^{-1} u^{0.34} e^{-u}$	$u = 13.6/T_e$	22
24	$O^+ + H \rightarrow O + H^+$	$k_{24} = 4.99 \times 10^{-11} T^{0.405} + 7.54 \times 10^{-10} T^{-0.458}$		23
25	$O + H^+ \rightarrow O^+ + H$	$k_{25} = [1.08 \times 10^{-11} T^{0.517}$		24
		$+ 4.00 \times 10^{-10} T^{0.00669}] \exp\left(-\frac{227}{T}\right)$		
26	$O + He^+ \rightarrow O^+ + He$	$k_{26} = 4.991 \times 10^{-15} \left(\frac{T}{10000}\right)^{0.3794} \exp\left(-\frac{T}{1121000}\right)$		25
		$+ 2.780 \times 10^{-15} \left(\frac{T}{10000}\right)^{-0.2163} \exp\left(\frac{T}{815800}\right)$		
27	$C + H^+ \rightarrow C^+ + H$	$k_{27} = 3.9 \times 10^{-16} T^{0.213}$		24
28	$C^+ + H \rightarrow C + H^+$	$k_{28} = 6.08 \times 10^{-14} \left(\frac{T}{10000}\right)^{1.96} \exp\left(-\frac{170000}{T}\right)$		24
29	$C + He^+ \rightarrow C^+ + He$	$k_{29} = 8.58 \times 10^{-17} T^{0.757}$	$T \leqslant 200$ K	26
		$= 3.25 \times 10^{-17} T^{0.968}$	$200 < T \leqslant 2000$ K	
		$= 2.77 \times 10^{-19} T^{1.597}$	$T > 2000$ K	
30	$H_2 + He \rightarrow H + H + He$	$k_{30,l} = \text{dex}[-27.029 + 3.801 \log(T) - 29487/T]$		27
		$k_{30,h} = \text{dex}[-2.729 - 1.75 \log(T) - 23474/T]$		
		$n_{cr,He} = \text{dex}\left[5.0792(1.0 - 1.23 \times 10^{-5} (T - 2000)\right]$		27
31	$OH + H \rightarrow O + H + H$	$k_{31} = 6.0 \times 10^{-9} \exp\left(-\frac{50900}{T}\right)$		28
32	$HOC^+ + H_2 \rightarrow HCO^+ + H_2$	$k_{32} = 3.8 \times 10^{-10}$		29
33	$HOC^+ + CO \rightarrow HCO^+ + CO$	$k_{33} = 4.0 \times 10^{-10}$		30
34	$C + H_2 \rightarrow CH + H$	$k_{34} = 6.64 \times 10^{-10} \exp\left(-\frac{11700}{T}\right)$		31
35	$CH + H \rightarrow C + H_2$	$k_{35} = 1.31 \times 10^{-10} \exp\left(-\frac{80}{T}\right)$		32

chemical model 2

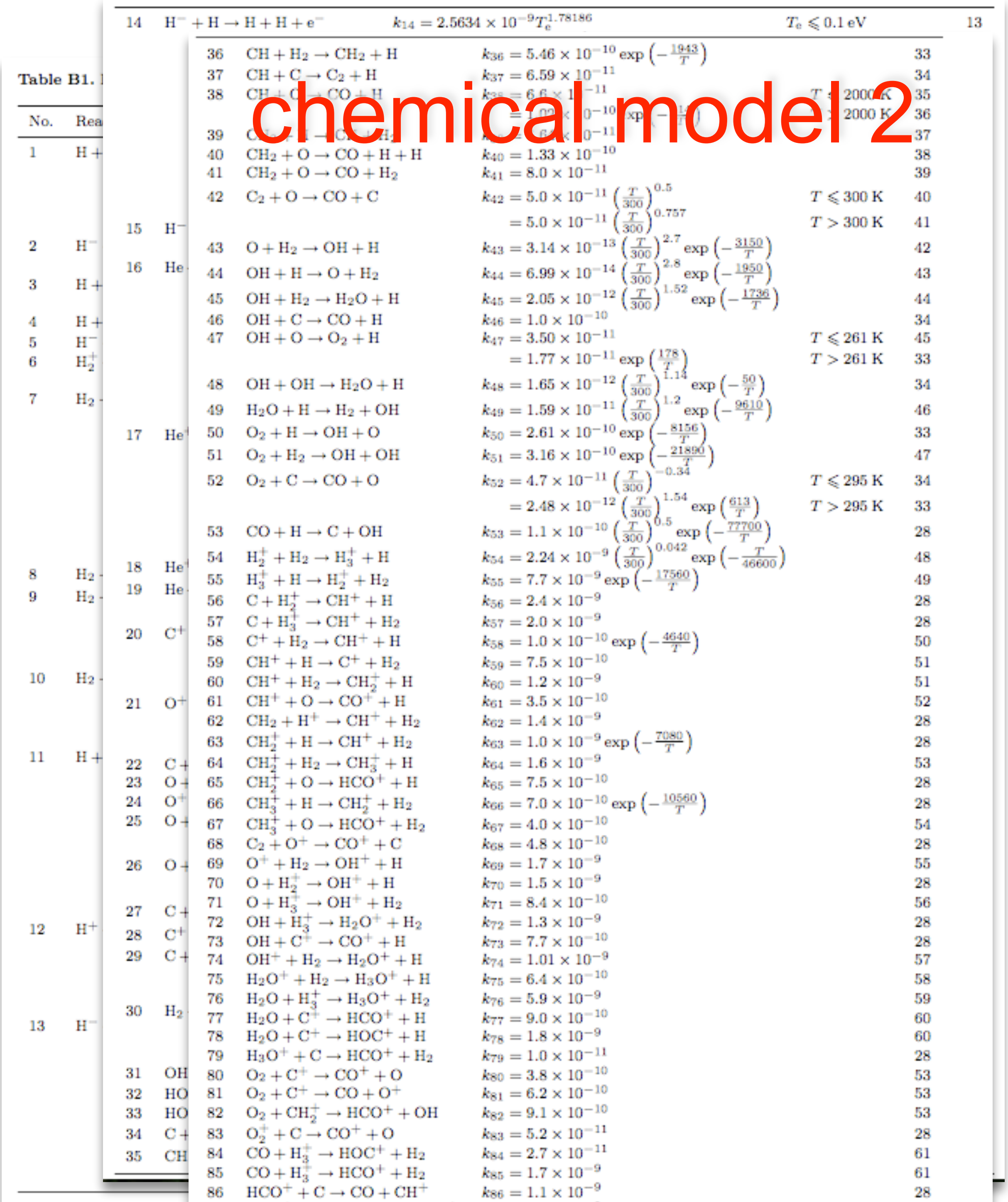


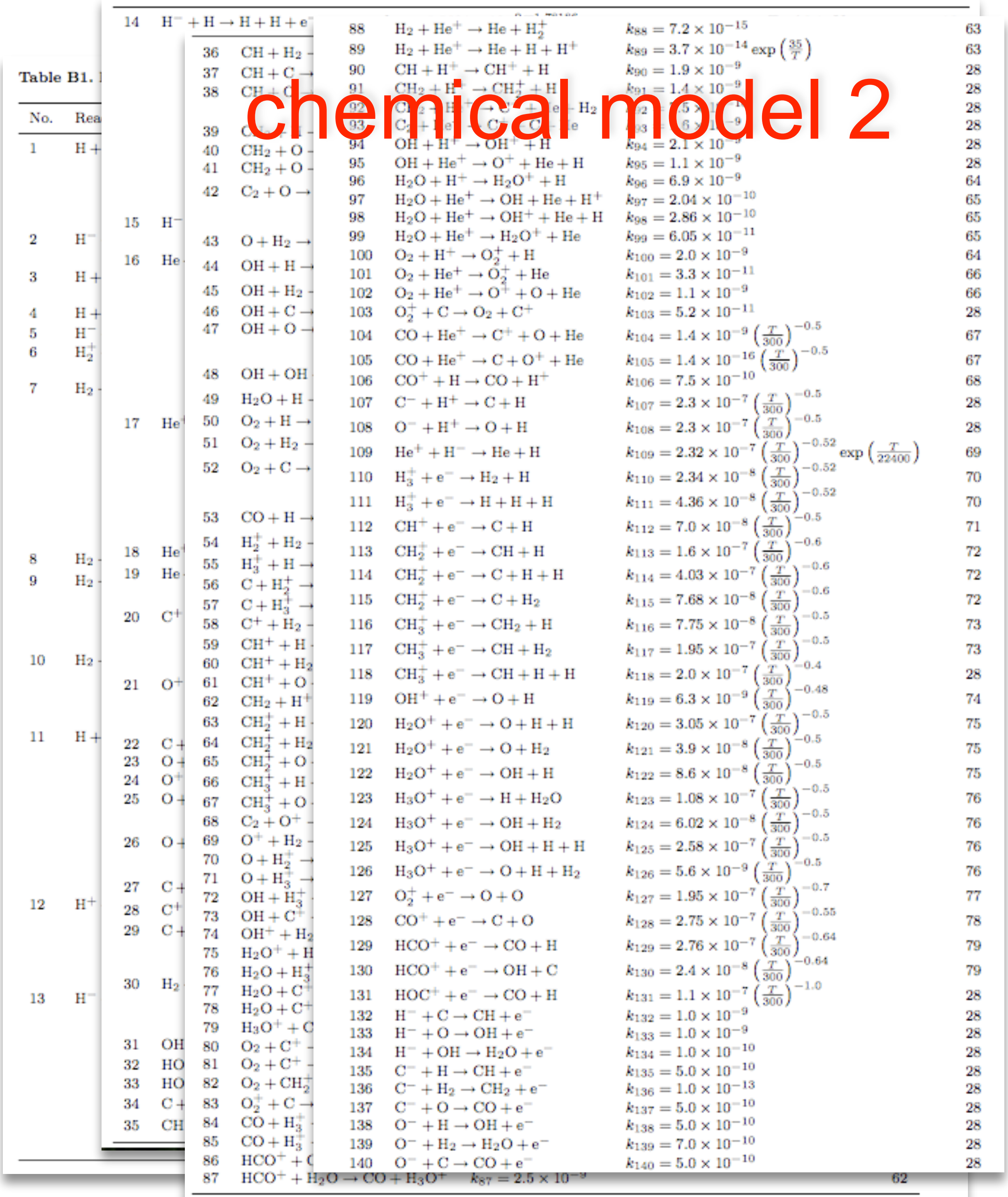
Table B1.

14	$H^- + H \rightarrow H + H + e^-$	$k_{14} = 2.5634 \times 10^{-9} T_e^{1.78186}$	$T_e \leqslant 0.1$ eV	13

36	$CH + H_2 \rightarrow CH_2 + H$	$k_{36} = 5.46 \times 10^{-10} \exp\left(-\frac{1943}{T}\right)$		33
37	$CH + C \rightarrow C_2 + H$	$k_{37} = 6.59 \times 10^{-11}$		34
38	$CH + O \rightarrow CO + H$	$k_{38} = 6.6 \times 10^{-11}$	$T \leqslant 2000$ K	35
		$= 1.02 \times 10^{-10} \exp\left(-\frac{[illegible]}{T}\right)$	$T > 2000$ K	36
39	$CH_2 + H \rightarrow CH + H_2$	$k_{39} = 6.$[illegible]$\times 10^{-11}$		37
40	$CH_2 + O \rightarrow CO + H + H$	$k_{40} = 1.33 \times 10^{-10}$		38
41	$CH_2 + O \rightarrow CO + H_2$	$k_{41} = 8.0 \times 10^{-11}$		39
42	$C_2 + O \rightarrow CO + C$	$k_{42} = 5.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.5}$	$T \leqslant 300$ K	40
		$= 5.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.757}$	$T > 300$ K	41
43	$O + H_2 \rightarrow OH + H$	$k_{43} = 3.14 \times 10^{-13} \left(\frac{T}{300}\right)^{2.7} \exp\left(-\frac{3150}{T}\right)$		42
44	$OH + H \rightarrow O + H_2$	$k_{44} = 6.99 \times 10^{-14} \left(\frac{T}{300}\right)^{2.8} \exp\left(-\frac{1950}{T}\right)$		43
45	$OH + H_2 \rightarrow H_2O + H$	$k_{45} = 2.05 \times 10^{-12} \left(\frac{T}{300}\right)^{1.52} \exp\left(-\frac{1736}{T}\right)$		44
46	$OH + C \rightarrow CO + H$	$k_{46} = 1.0 \times 10^{-10}$		34
47	$OH + O \rightarrow O_2 + H$	$k_{47} = 3.50 \times 10^{-11}$	$T \leqslant 261$ K	45
		$= 1.77 \times 10^{-11} \exp\left(\frac{178}{T}\right)$	$T > 261$ K	33
48	$OH + OH \rightarrow H_2O + H$	$k_{48} = 1.65 \times 10^{-12} \left(\frac{T}{300}\right)^{1.14} \exp\left(-\frac{50}{T}\right)$		34
49	$H_2O + H \rightarrow H_2 + OH$	$k_{49} = 1.59 \times 10^{-11} \left(\frac{T}{300}\right)^{1.2} \exp\left(-\frac{9610}{T}\right)$		46
50	$O_2 + H \rightarrow OH + O$	$k_{50} = 2.61 \times 10^{-10} \exp\left(-\frac{8156}{T}\right)$		33
51	$O_2 + H_2 \rightarrow OH + OH$	$k_{51} = 3.16 \times 10^{-10} \exp\left(-\frac{21890}{T}\right)$		47
52	$O_2 + C \rightarrow CO + O$	$k_{52} = 4.7 \times 10^{-11} \left(\frac{T}{300}\right)^{-0.34}$	$T \leqslant 295$ K	34
		$= 2.48 \times 10^{-12} \left(\frac{T}{300}\right)^{1.54} \exp\left(\frac{613}{T}\right)$	$T > 295$ K	33
53	$CO + H \rightarrow C + OH$	$k_{53} = 1.1 \times 10^{-10} \left(\frac{T}{300}\right)^{0.5} \exp\left(-\frac{77700}{T}\right)$		28
54	$H_2^+ + H_2 \rightarrow H_3^+ + H$	$k_{54} = 2.24 \times 10^{-9} \left(\frac{T}{300}\right)^{0.042} \exp\left(-\frac{T}{46600}\right)$		48
55	$H_3^+ + H \rightarrow H_2^+ + H_2$	$k_{55} = 7.7 \times 10^{-9} \exp\left(-\frac{17560}{T}\right)$		49
56	$C + H_2^+ \rightarrow CH^+ + H$	$k_{56} = 2.4 \times 10^{-9}$		28
57	$C + H_3^+ \rightarrow CH^+ + H_2$	$k_{57} = 2.0 \times 10^{-9}$		28
58	$C^+ + H_2 \rightarrow CH^+ + H$	$k_{58} = 1.0 \times 10^{-10} \exp\left(-\frac{4640}{T}\right)$		50
59	$CH^+ + H \rightarrow C^+ + H_2$	$k_{59} = 7.5 \times 10^{-10}$		51
60	$CH^+ + H_2 \rightarrow CH_2^+ + H$	$k_{60} = 1.2 \times 10^{-9}$		51
61	$CH^+ + O \rightarrow CO^+ + H$	$k_{61} = 3.5 \times 10^{-10}$		52
62	$CH_2 + H^+ \rightarrow CH^+ + H_2$	$k_{62} = 1.4 \times 10^{-9}$		28
63	$CH_2^+ + H \rightarrow CH^+ + H_2$	$k_{63} = 1.0 \times 10^{-9} \exp\left(-\frac{7080}{T}\right)$		28
64	$CH_2^+ + H_2 \rightarrow CH_3^+ + H$	$k_{64} = 1.6 \times 10^{-9}$		53
65	$CH_2^+ + O \rightarrow HCO^+ + H$	$k_{65} = 7.5 \times 10^{-10}$		28
66	$CH_3^+ + H \rightarrow CH_2^+ + H_2$	$k_{66} = 7.0 \times 10^{-10} \exp\left(-\frac{10560}{T}\right)$		28
67	$CH_3^+ + O \rightarrow HCO^+ + H_2$	$k_{67} = 4.0 \times 10^{-10}$		54
68	$C_2 + O^+ \rightarrow CO^+ + C$	$k_{68} = 4.8 \times 10^{-10}$		28
69	$O^+ + H_2 \rightarrow OH^+ + H$	$k_{69} = 1.7 \times 10^{-9}$		55
70	$O + H_2^+ \rightarrow OH^+ + H$	$k_{70} = 1.5 \times 10^{-9}$		28
71	$O + H_3^+ \rightarrow OH^+ + H_2$	$k_{71} = 8.4 \times 10^{-10}$		56
72	$OH + H_3^+ \rightarrow H_2O^+ + H_2$	$k_{72} = 1.3 \times 10^{-9}$		28
73	$OH + C^+ \rightarrow CO^+ + H$	$k_{73} = 7.7 \times 10^{-10}$		28
74	$OH^+ + H_2 \rightarrow H_2O^+ + H$	$k_{74} = 1.01 \times 10^{-9}$		57
75	$H_2O^+ + H_2 \rightarrow H_3O^+ + H$	$k_{75} = 6.4 \times 10^{-10}$		58
76	$H_2O + H_3^+ \rightarrow H_3O^+ + H_2$	$k_{76} = 5.9 \times 10^{-9}$		59
77	$H_2O + C^+ \rightarrow HCO^+ + H$	$k_{77} = 9.0 \times 10^{-10}$		60
78	$H_2O + C^+ \rightarrow HOC^+ + H$	$k_{78} = 1.8 \times 10^{-9}$		60
79	$H_3O^+ + C \rightarrow HCO^+ + H_2$	$k_{79} = 1.0 \times 10^{-11}$		28
80	$O_2 + C^+ \rightarrow CO^+ + O$	$k_{80} = 3.8 \times 10^{-10}$		53
81	$O_2 + C^+ \rightarrow CO + O^+$	$k_{81} = 6.2 \times 10^{-10}$		53
82	$O_2 + CH_2^+ \rightarrow HCO^+ + OH$	$k_{82} = 9.1 \times 10^{-10}$		53
83	$O_2^+ + C \rightarrow CO^+ + O$	$k_{83} = 5.2 \times 10^{-11}$		28
84	$CO + H_3^+ \rightarrow HOC^+ + H_2$	$k_{84} = 2.7 \times 10^{-11}$		61
85	$CO + H_3^+ \rightarrow HCO^+ + H_2$	$k_{85} = 1.7 \times 10^{-9}$		61
86	$HCO^+ + C \rightarrow CO + CH^+$	$k_{86} = 1.1 \times 10^{-9}$		28
87	$HCO^+ + H_2O \rightarrow CO + H_3O^+$	$k_{87} = 2.5 \times 10^{-9}$		62

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

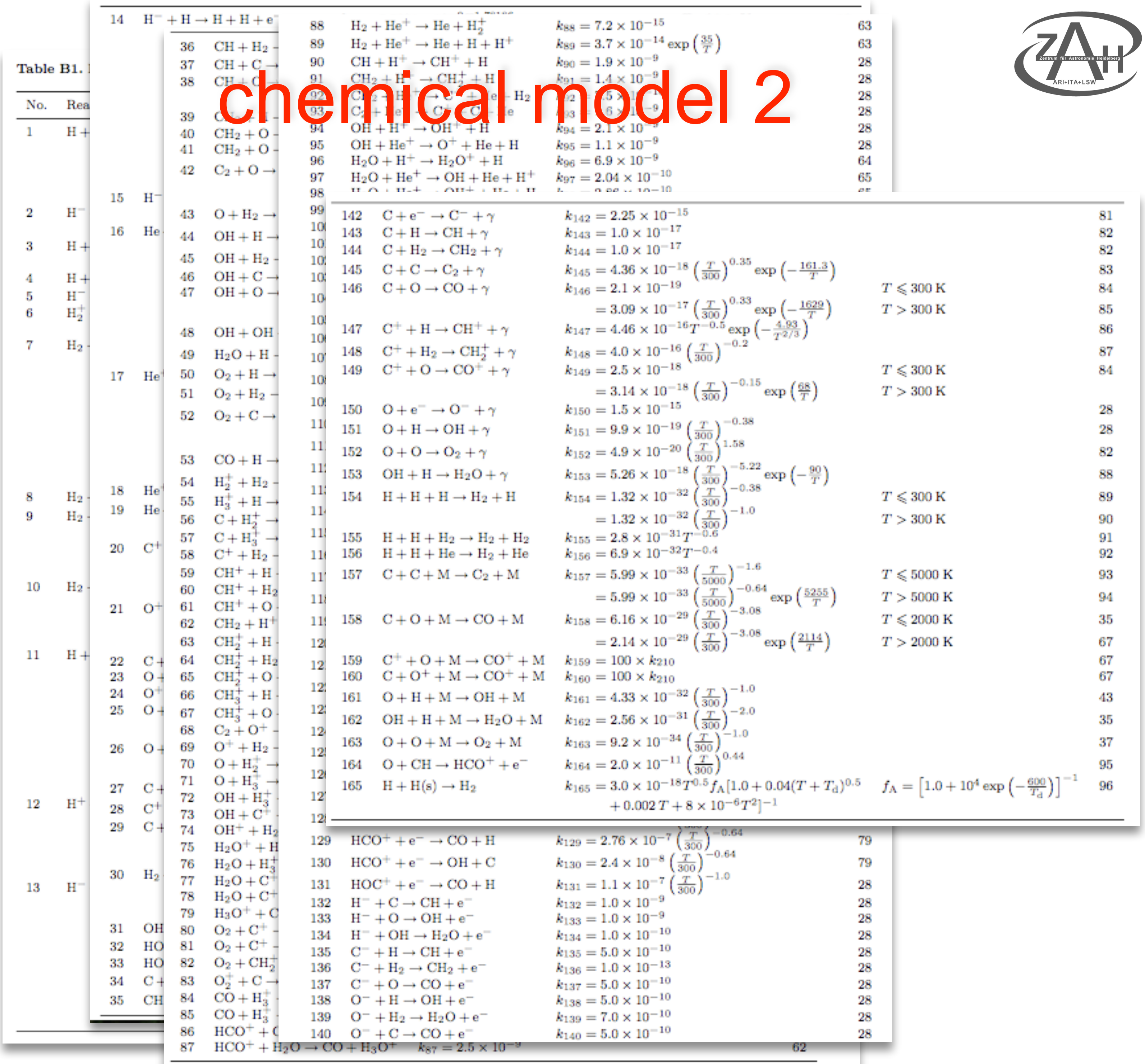
chemical model 2



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

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

chemical model 2



88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$		63
89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$		63
90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$		28
91	$CH_2 + H^+ \rightarrow CH_2^+ + H$	$k_{91} = 1.4 \times 10^{-9}$		28
92	[illegible] $\rightarrow C^+ +$ [illegible] $+ H_2$	[illegible]		28
93	$C_2 +$ [illegible]	[illegible]		28
94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-9}$		28
95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$		28
96	$H_2O + H^+ \rightarrow H_2O^+ + H$	$k_{96} = 6.9 \times 10^{-9}$		64
97	$H_2O + He^+ \rightarrow OH + He + H^+$	$k_{97} = 2.04 \times 10^{-10}$		65

142	$C + e^- \rightarrow C^- + \gamma$	$k_{142} = 2.25 \times 10^{-15}$		81
143	$C + H \rightarrow CH + \gamma$	$k_{143} = 1.0 \times 10^{-17}$		82
144	$C + H_2 \rightarrow CH_2 + \gamma$	$k_{144} = 1.0 \times 10^{-17}$		82
145	$C + C \rightarrow C_2 + \gamma$	$k_{145} = 4.36 \times 10^{-18} \left(\frac{T}{300}\right)^{0.35} \exp\left(-\frac{161.3}{T}\right)$		83
146	$C + O \rightarrow CO + \gamma$	$k_{146} = 2.1 \times 10^{-19}$	$T \leqslant 300$ K	84
		$= 3.09 \times 10^{-17} \left(\frac{T}{300}\right)^{0.33} \exp\left(-\frac{1629}{T}\right)$	$T > 300$ K	85
147	$C^+ + H \rightarrow CH^+ + \gamma$	$k_{147} = 4.46 \times 10^{-16} T^{-0.5} \exp\left(-\frac{4.93}{T^{2/3}}\right)$		86
148	$C^+ + H_2 \rightarrow CH_2^+ + \gamma$	$k_{148} = 4.0 \times 10^{-16} \left(\frac{T}{300}\right)^{-0.2}$		87
149	$C^+ + O \rightarrow CO^+ + \gamma$	$k_{149} = 2.5 \times 10^{-18}$	$T \leqslant 300$ K	84
		$= 3.14 \times 10^{-18} \left(\frac{T}{300}\right)^{-0.15} \exp\left(\frac{68}{T}\right)$	$T > 300$ K	
150	$O + e^- \rightarrow O^- + \gamma$	$k_{150} = 1.5 \times 10^{-15}$		28
151	$O + H \rightarrow OH + \gamma$	$k_{151} = 9.9 \times 10^{-19} \left(\frac{T}{300}\right)^{-0.38}$		28
152	$O + O \rightarrow O_2 + \gamma$	$k_{152} = 4.9 \times 10^{-20} \left(\frac{T}{300}\right)^{1.58}$		82
153	$OH + H \rightarrow H_2O + \gamma$	$k_{153} = 5.26 \times 10^{-18} \left(\frac{T}{300}\right)^{-5.22} \exp\left(-\frac{90}{T}\right)$		88
154	$H + H + H \rightarrow H_2 + H$	$k_{154} = 1.32 \times 10^{-32} \left(\frac{T}{300}\right)^{-0.38}$	$T \leqslant 300$ K	89
		$= 1.32 \times 10^{-32} \left(\frac{T}{300}\right)^{-1.0}$	$T > 300$ K	90
155	$H + H + H_2 \rightarrow H_2 + H_2$	$k_{155} = 2.8 \times 10^{-31} T^{-0.6}$		91
156	$H + H + He \rightarrow H_2 + He$	$k_{156} = 6.9 \times 10^{-32} T^{-0.4}$		92
157	$C + C + M \rightarrow C_2 + M$	$k_{157} = 5.99 \times 10^{-33} \left(\frac{T}{5000}\right)^{-1.6}$	$T \leqslant 5000$ K	93
		$= 5.99 \times 10^{-33} \left(\frac{T}{5000}\right)^{-0.64} \exp\left(\frac{5255}{T}\right)$	$T > 5000$ K	94
158	$C + O + M \rightarrow CO + M$	$k_{158} = 6.16 \times 10^{-29} \left(\frac{T}{300}\right)^{-3.08}$	$T \leqslant 2000$ K	35
		$= 2.14 \times 10^{-29} \left(\frac{T}{300}\right)^{-3.08} \exp\left(\frac{2114}{T}\right)$	$T > 2000$ K	67
159	$C^+ + O + M \rightarrow CO^+ + M$	$k_{159} = 100 \times k_{210}$		67
160	$C + O^+ + M \rightarrow CO^+ + M$	$k_{160} = 100 \times k_{210}$		67
161	$O + H + M \rightarrow OH + M$	$k_{161} = 4.33 \times 10^{-32} \left(\frac{T}{300}\right)^{-1.0}$		43
162	$OH + H + M \rightarrow H_2O + M$	$k_{162} = 2.56 \times 10^{-31} \left(\frac{T}{300}\right)^{-2.0}$		35
163	$O + O + M \rightarrow O_2 + M$	$k_{163} = 9.2 \times 10^{-34} \left(\frac{T}{300}\right)^{-1.0}$		37
164	$O + CH \rightarrow HCO^+ + e^-$	$k_{164} = 2.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.44}$		95
165	$H + H(s) \rightarrow H_2$	$k_{165} = 3.0 \times 10^{-18} T^{0.5} f_A [1.0 + 0.04(T + T_d)^{0.5}$ $+ 0.002\,T + 8 \times 10^{-6} T^2]^{-1}$	$f_A = \left[1.0 + 10^4 \exp\left(-\frac{600}{T_d}\right)\right]^{-1}$	96

129	$HCO^+ + e^- \rightarrow CO + H$	$k_{129} = 2.76 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.64}$	79
130	$HCO^+ + e^- \rightarrow OH + C$	$k_{130} = 2.4 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.64}$	79
131	$HOC^+ + e^- \rightarrow CO + H$	$k_{131} = 1.1 \times 10^{-7} \left(\frac{T}{300}\right)^{-1.0}$	28
132	$H^- + C \rightarrow CH + e^-$	$k_{132} = 1.0 \times 10^{-9}$	28
133	$H^- + O \rightarrow OH + e^-$	$k_{133} = 1.0 \times 10^{-9}$	28
134	$H^- + OH \rightarrow H_2O + e^-$	$k_{134} = 1.0 \times 10^{-10}$	28
135	$C^- + H \rightarrow CH + e^-$	$k_{135} = 5.0 \times 10^{-10}$	28
136	$C^- + H_2 \rightarrow CH_2 + e^-$	$k_{136} = 1.0 \times 10^{-13}$	28
137	$C^- + O \rightarrow CO + e^-$	$k_{137} = 5.0 \times 10^{-10}$	28
138	$O^- + H \rightarrow OH + e^-$	$k_{138} = 5.0 \times 10^{-10}$	28
139	$O^- + H_2 \rightarrow H_2O + e^-$	$k_{139} = 7.0 \times 10^{-10}$	28
140	$O^- + C \rightarrow CO + e^-$	$k_{140} = 5.0 \times 10^{-10}$	28

87 $HCO^+ + H_2O \rightarrow CO + H_3O^+$ $k_{87} = 2.5 \times 10^{-9}$ 62

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

chemical model 2

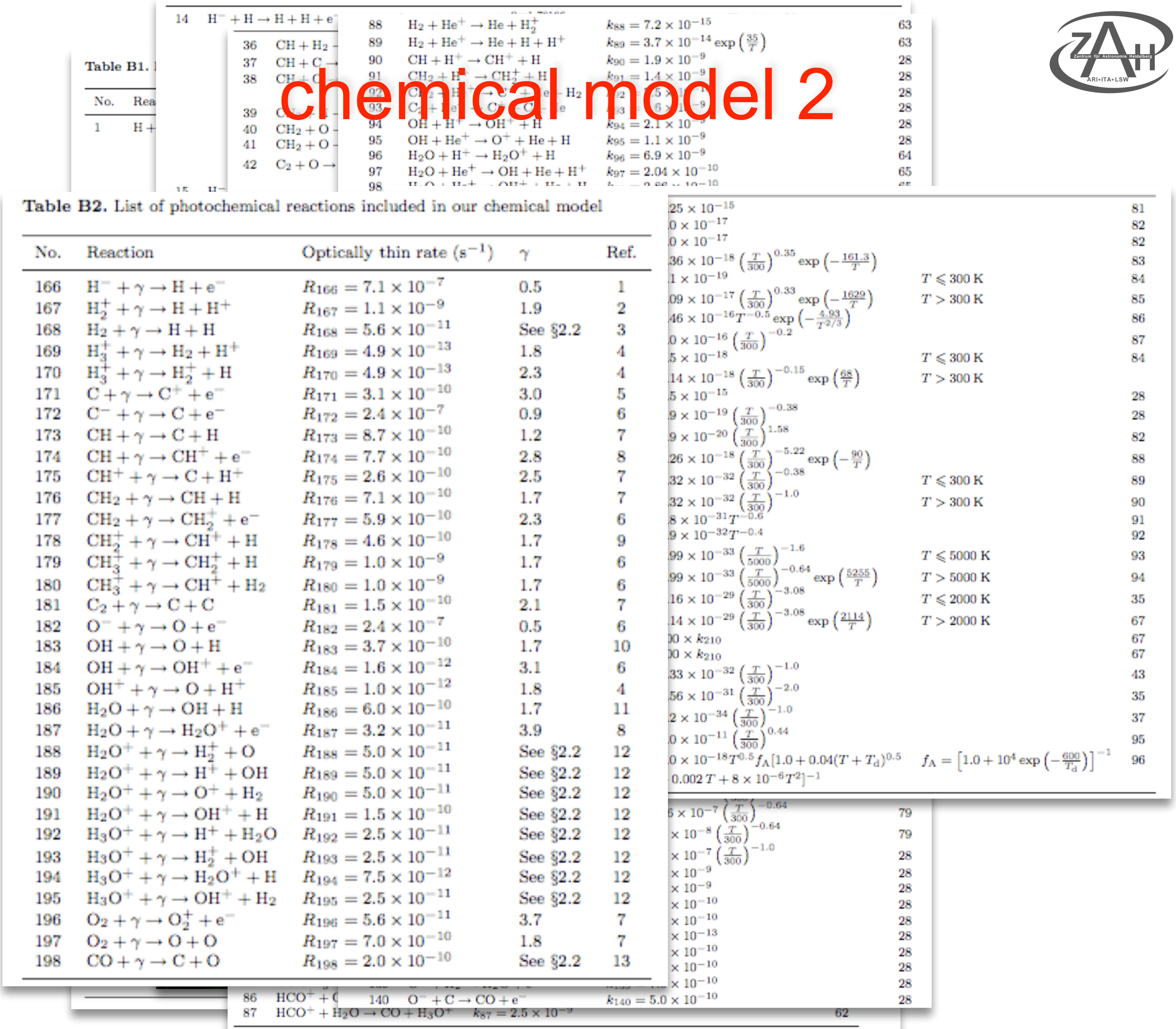
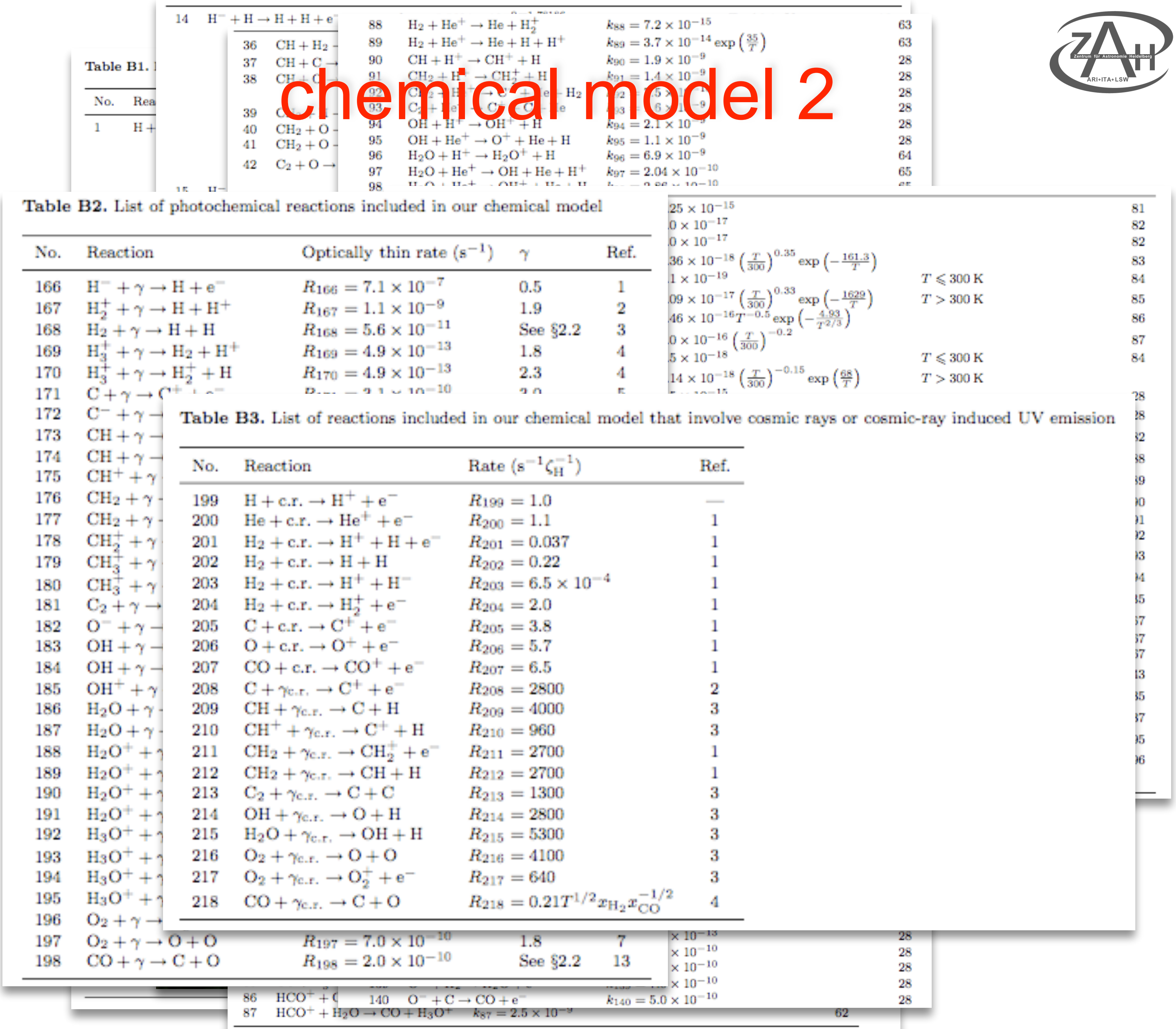


Table B2. List of photochemical reactions included in our chemical model

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

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

chemical model 2



88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$	63
89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$	63
90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$	28
91	$CH_2 + H^+ \rightarrow CH_2^+ + H$	$k_{91} = 1.4 \times 10^{-9}$	28
92	$CH_2 + He^+ \rightarrow C^+ + He + H_2$	[illegible]	28
93	$C_2 + He^+ \rightarrow C^+ + C + He$	[illegible]	28
94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10$	28
95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$	28
96	$H_2O + H^+ \rightarrow H_2O^+ + H$	$k_{96} = 6.9 \times 10^{-9}$	64
97	$H_2O + He^+ \rightarrow OH + He + H^+$	$k_{97} = 2.04 \times 10^{-10}$	65

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

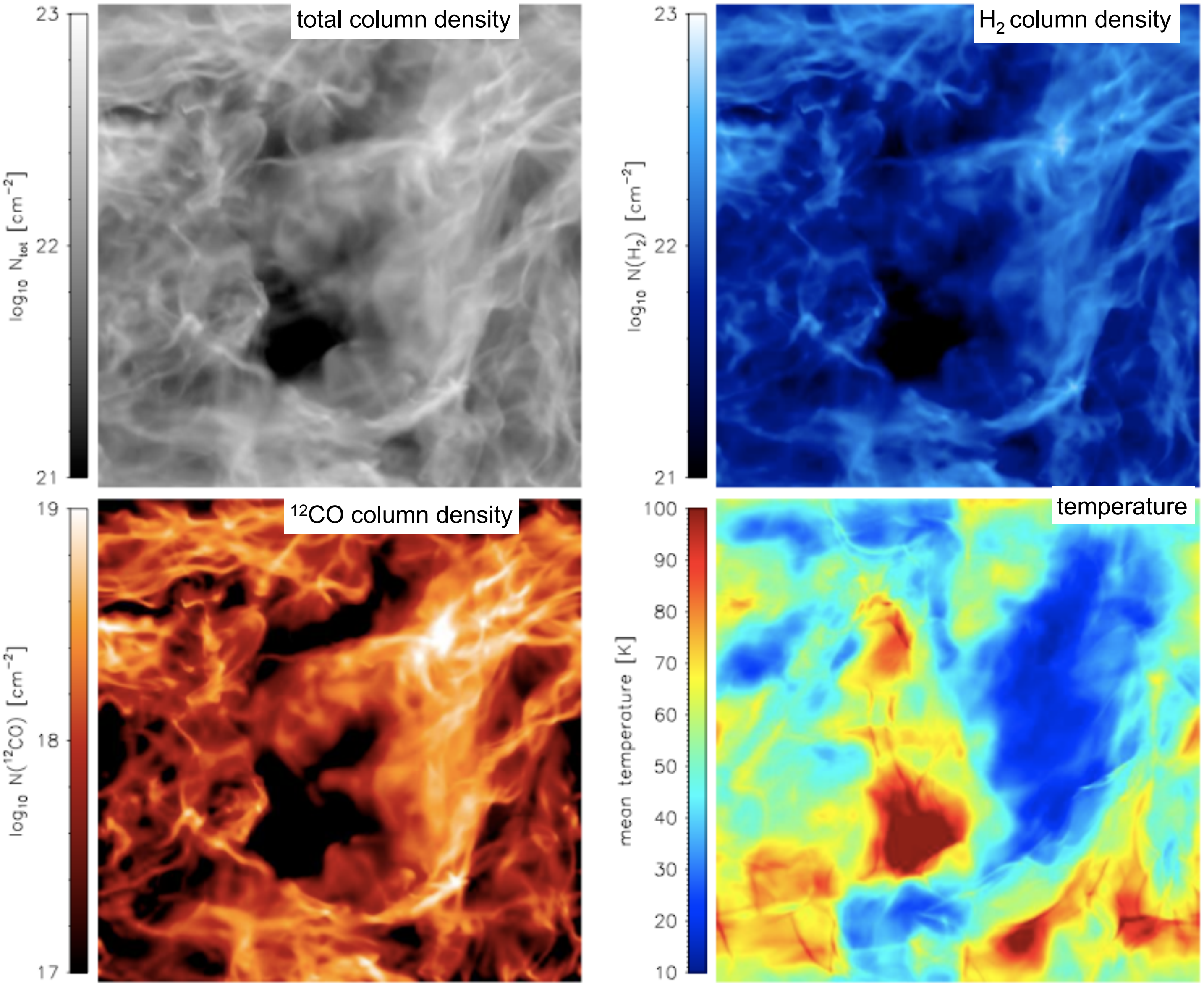
No.	Reaction	Optically thin rate (s^{-1})	γ	Ref.
166	$H^- + \gamma \rightarrow H + e^-$	$R_{166} = 7.1 \times 10^{-7}$	0.5	1
167	$H_2^+ + \gamma \rightarrow H + H^+$	$R_{167} = 1.1 \times 10^{-9}$	1.9	2
168	$H_2 + \gamma \rightarrow H + H$	$R_{168} = 5.6 \times 10^{-11}$	See §2.2	3
169	$H_3^+ + \gamma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

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

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

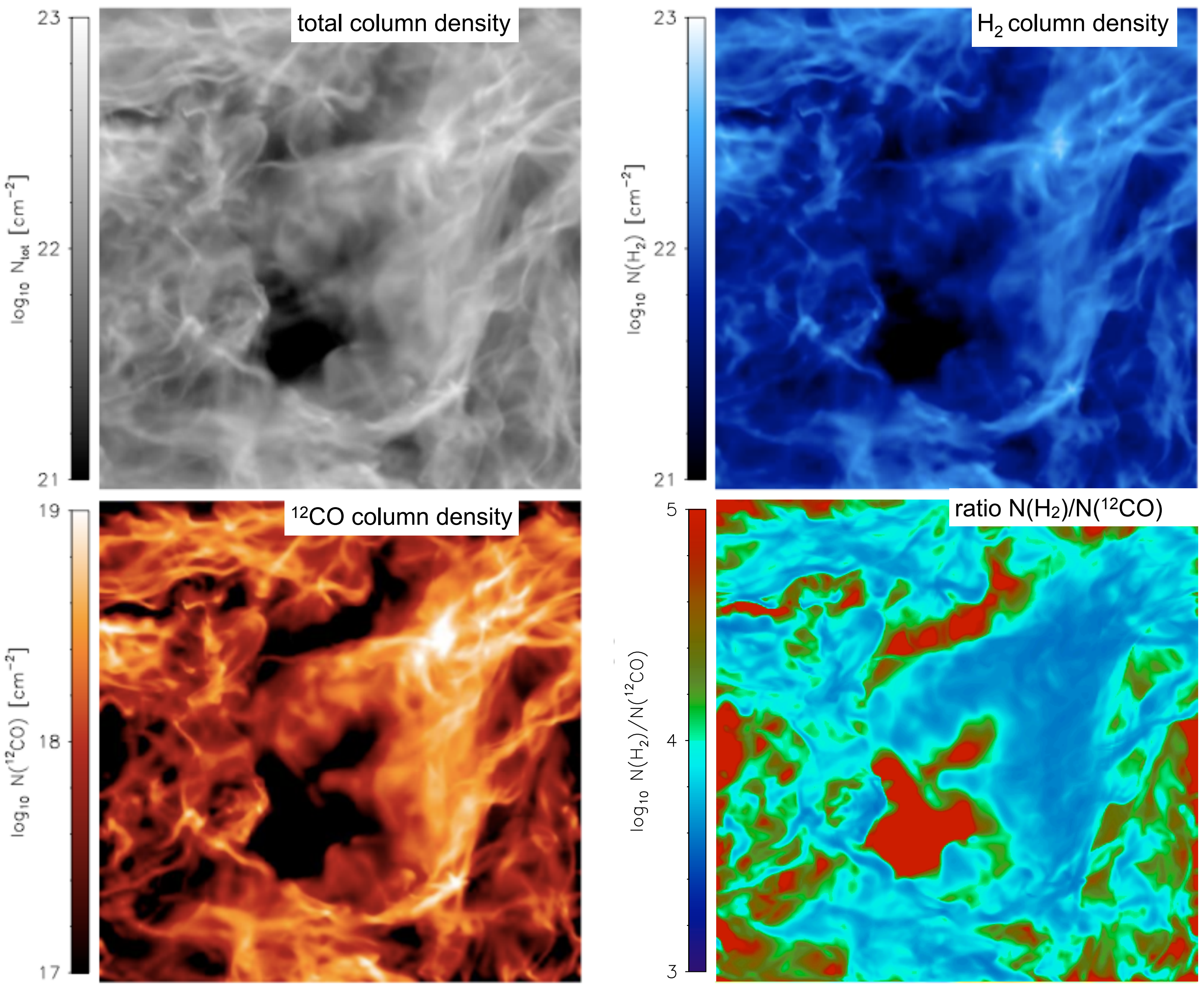
(Glover, Federrath, Mac Low, Klessen, 2010, MNRS, 404, 2)

effects of chemistry



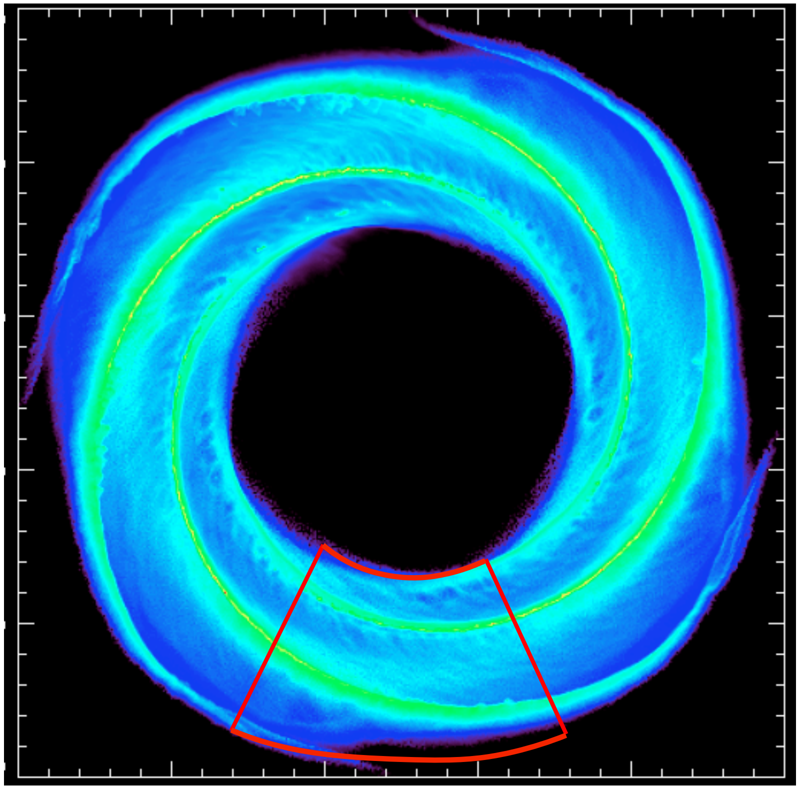
(Glover et al. 2010)

effects of chemistry



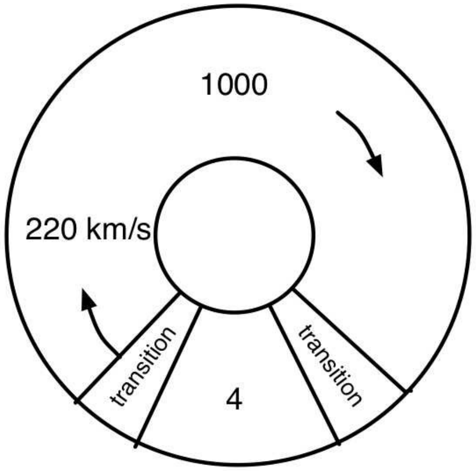
(Glover et al. 2010)

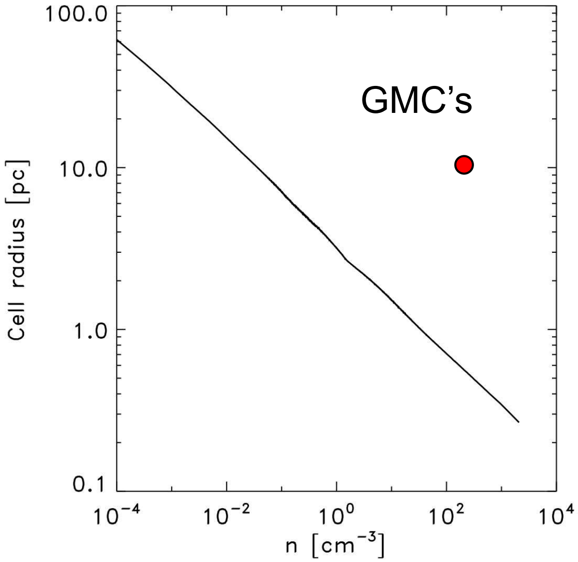
modeling molecular cloud formation



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

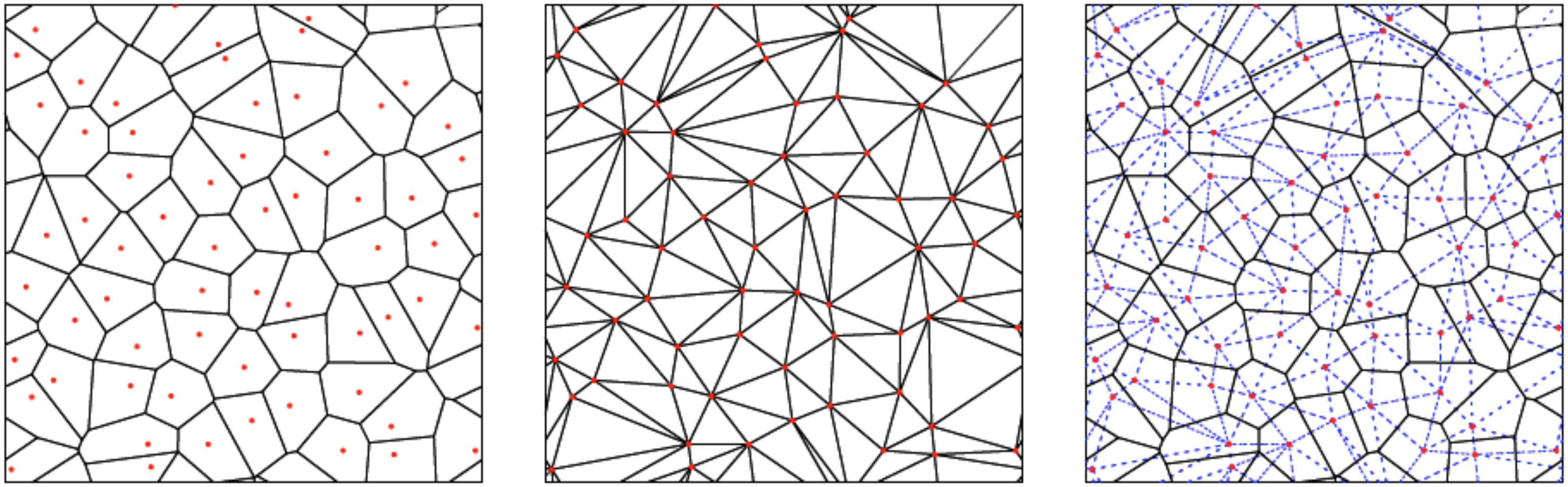
(Smith et al., 2014, MNRAS, 441, 1628)





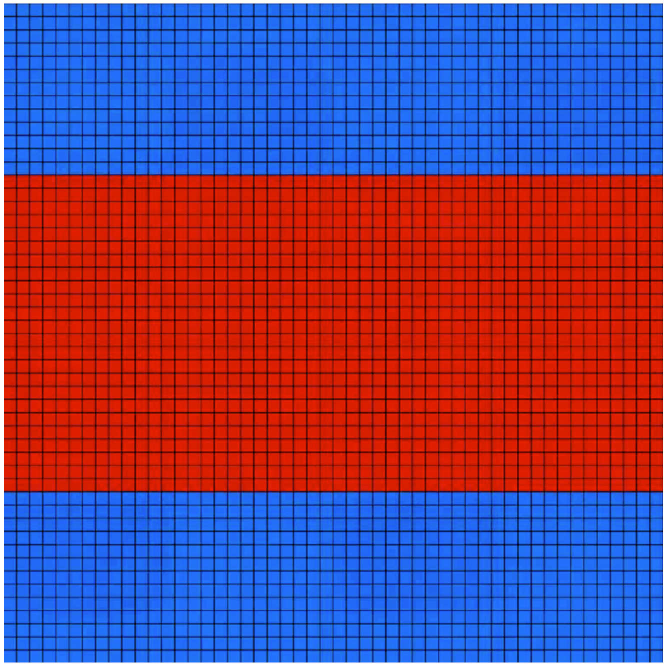
- Arepo moving mesh code *(Springel 2010)*
- time dependent chemistry *(Glover et al. 2007)* gives heating & cooling in a 2 phase medium
- two layers of refinement with mass resolution down to 4 $M_\odot$ in full Galaxy simulation
- UV field and cosmic rays
- TreeCol *(Clark et al. 2012)*
- external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

numerical method

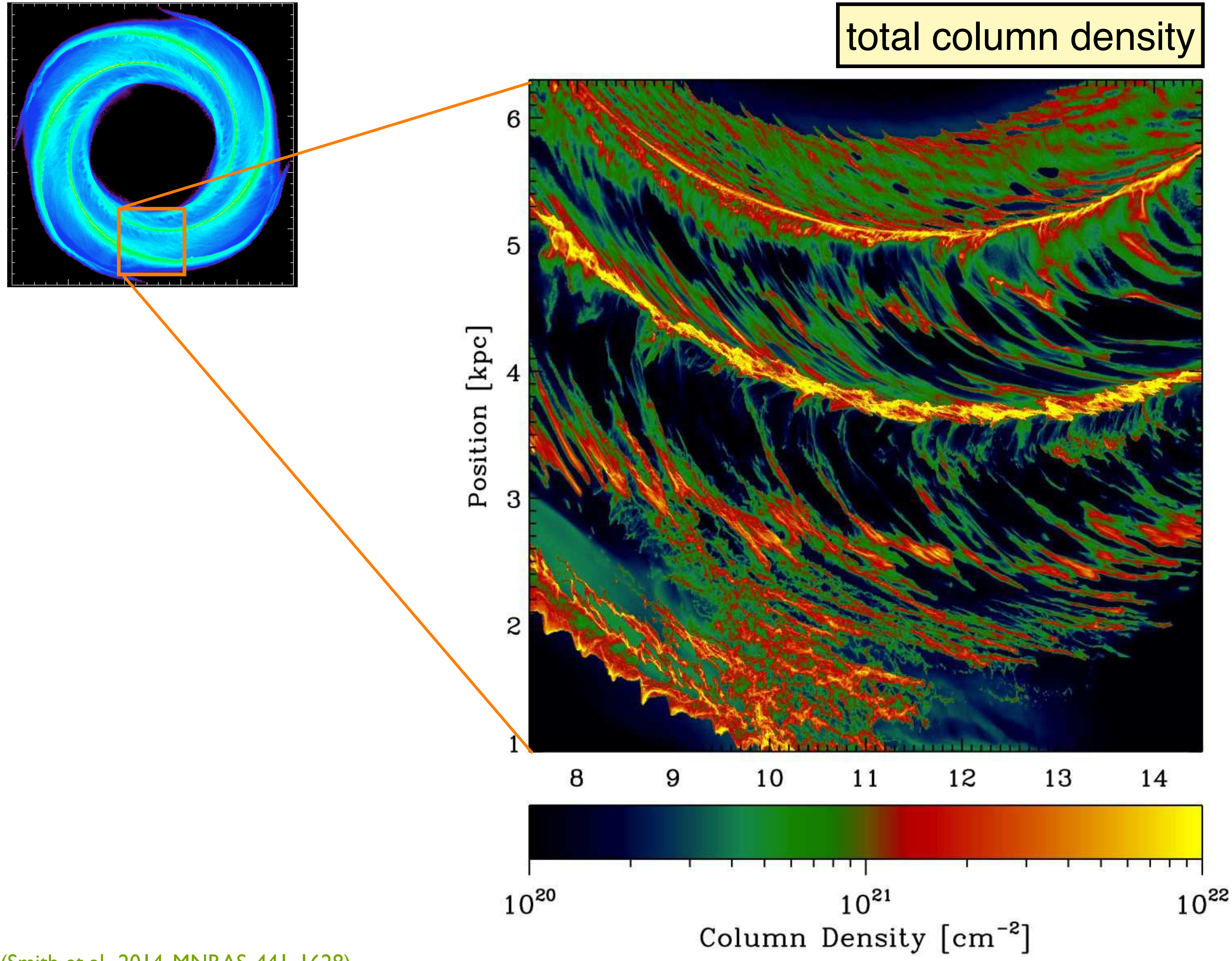


moving mesh code ***Arepo****:*

- 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

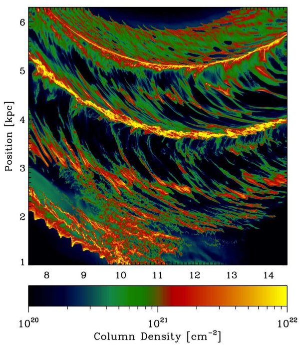


Springel (2010, MNRAS, 401, 791)

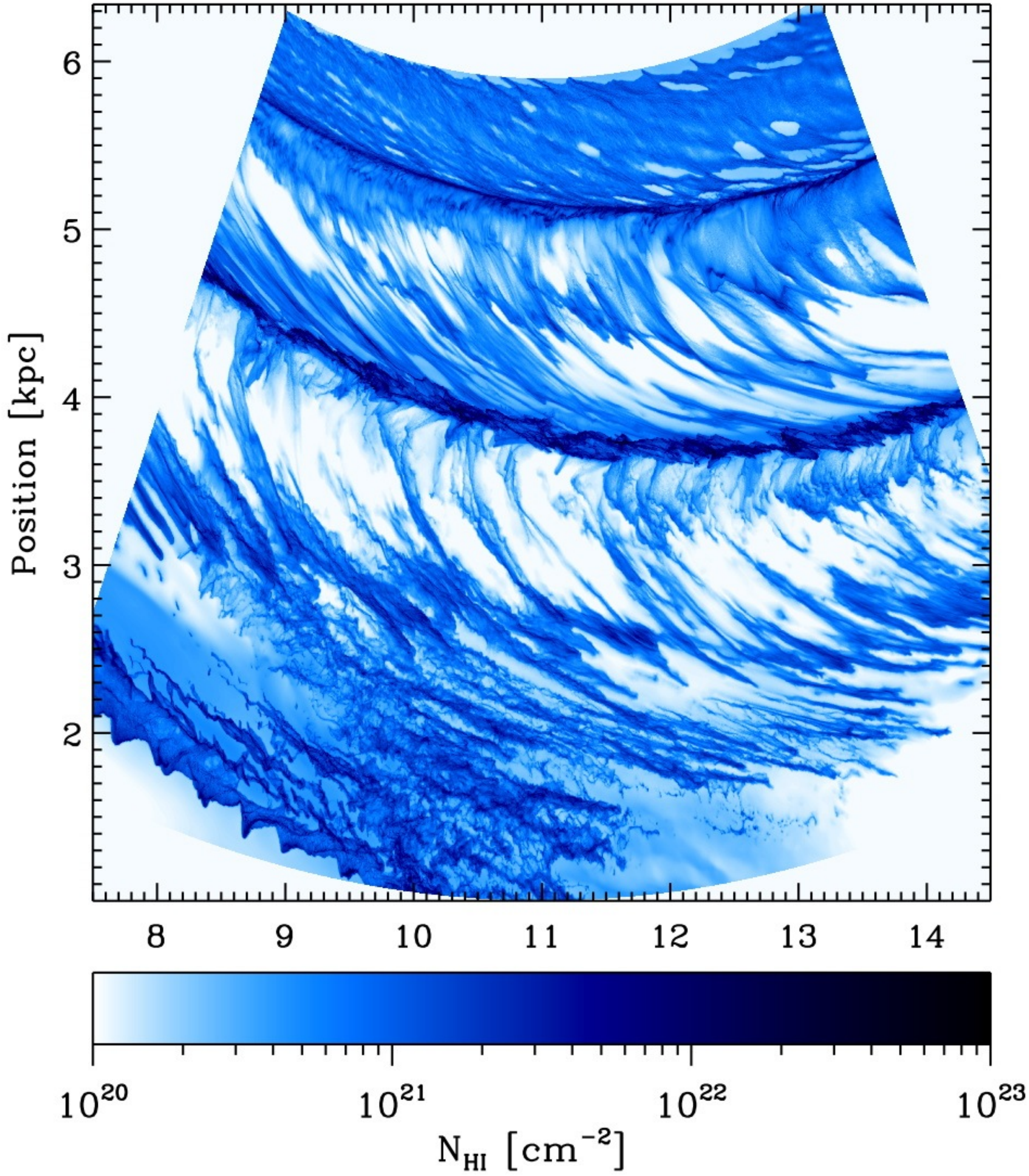


total column density

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

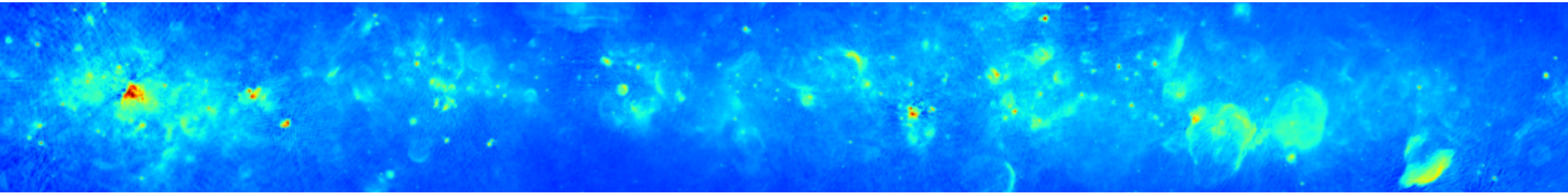


HI column density

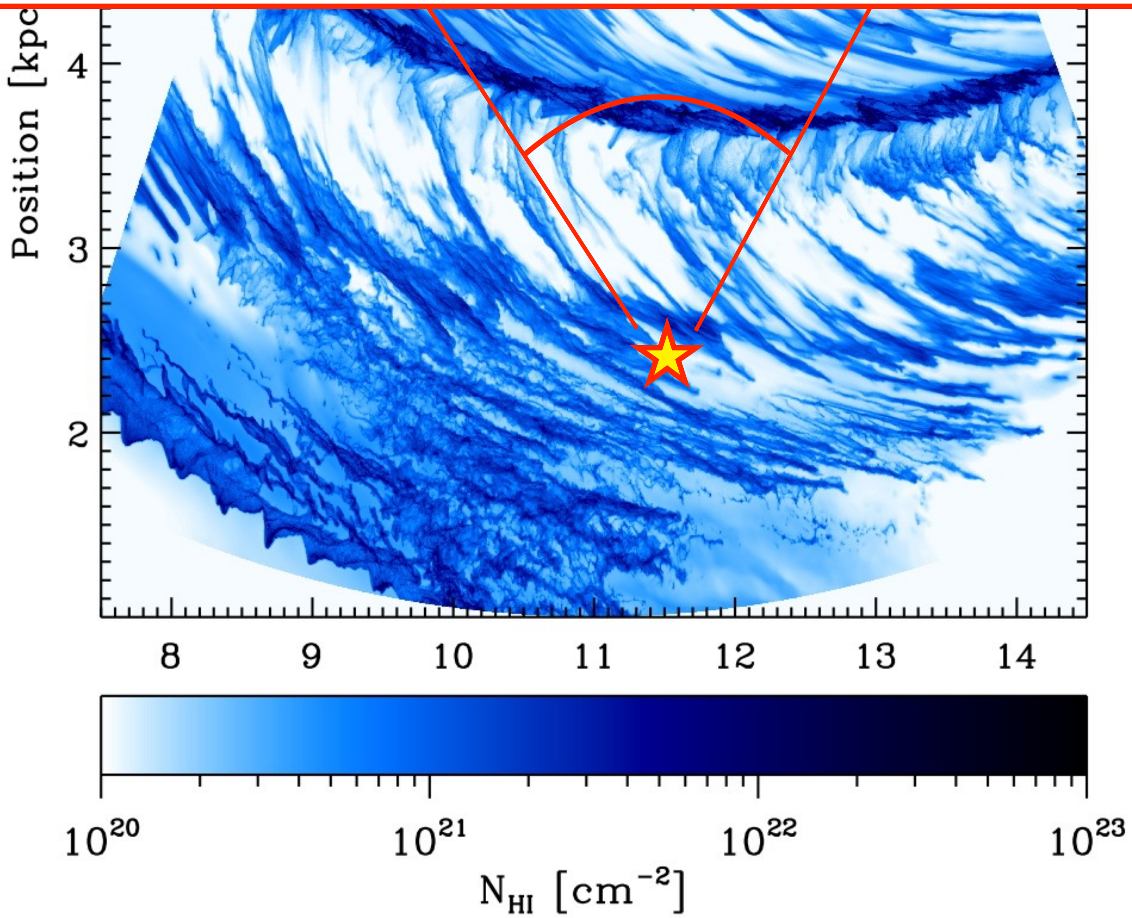


(Smith et al., 2014, MNRAS, 441, 1628)

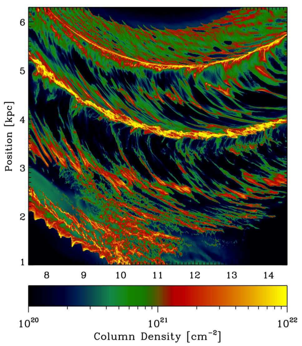
preliminary image from THOR Galactic plane survey (PI H. Beuther): continuum emission around 21 cm

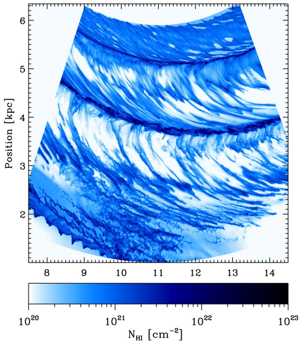


next step: produce all sky maps at various positions in the model galaxy (use RADMC-3D)

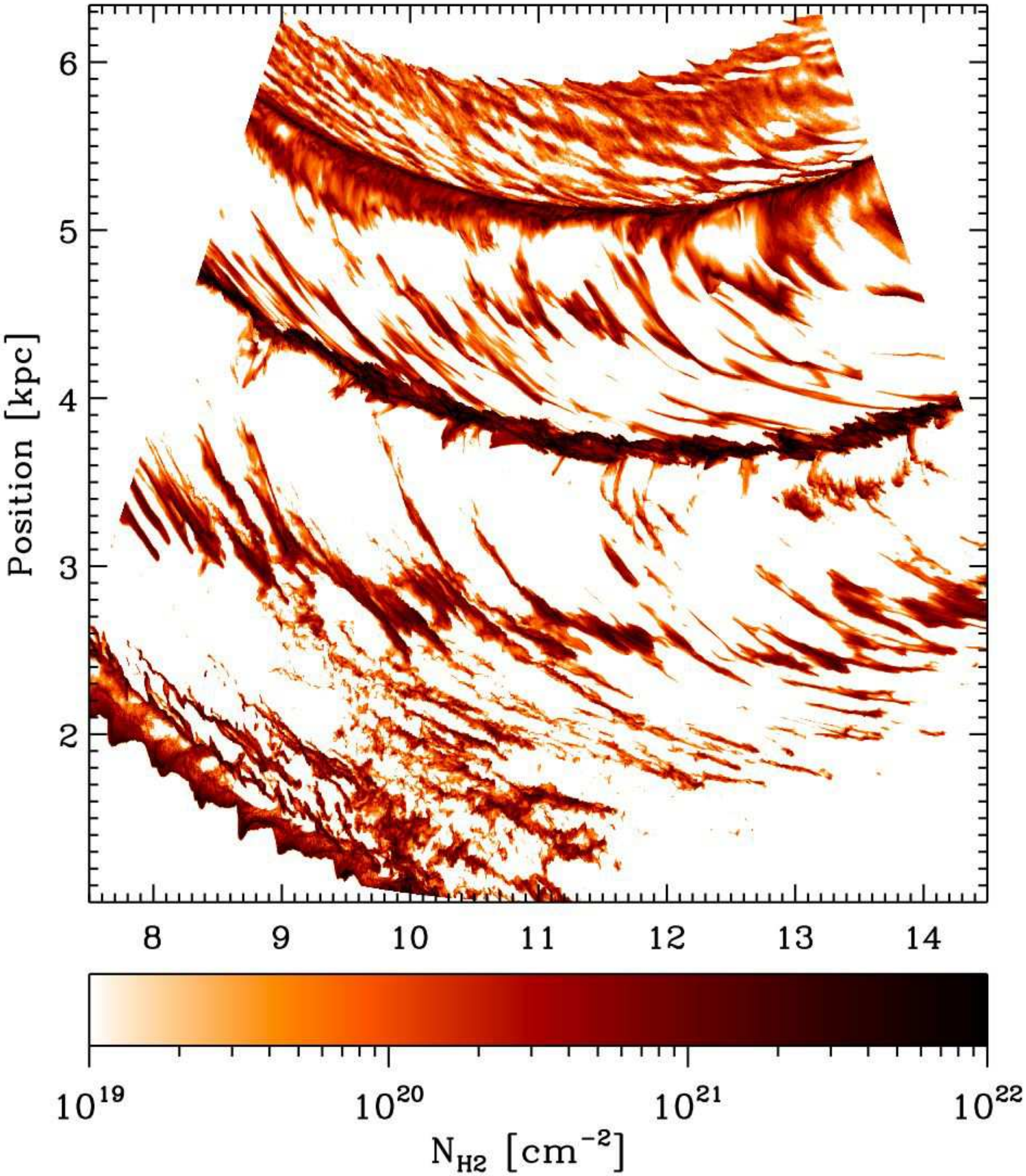


(Smith et al., 2014, MNRAS, 441, 1628)

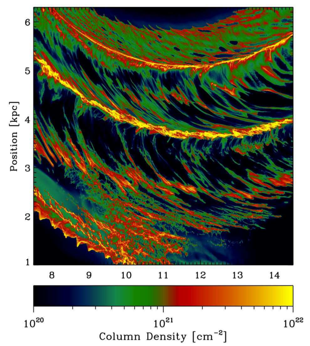


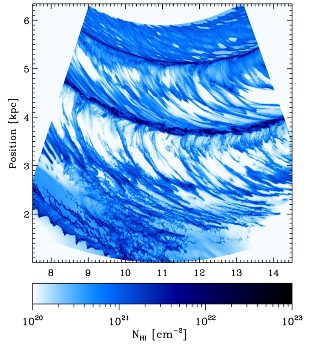


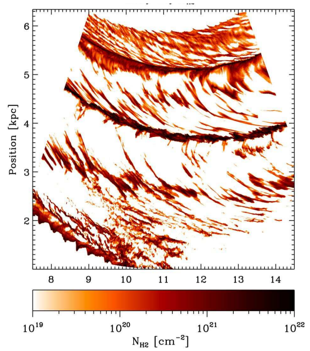
H_2 column density



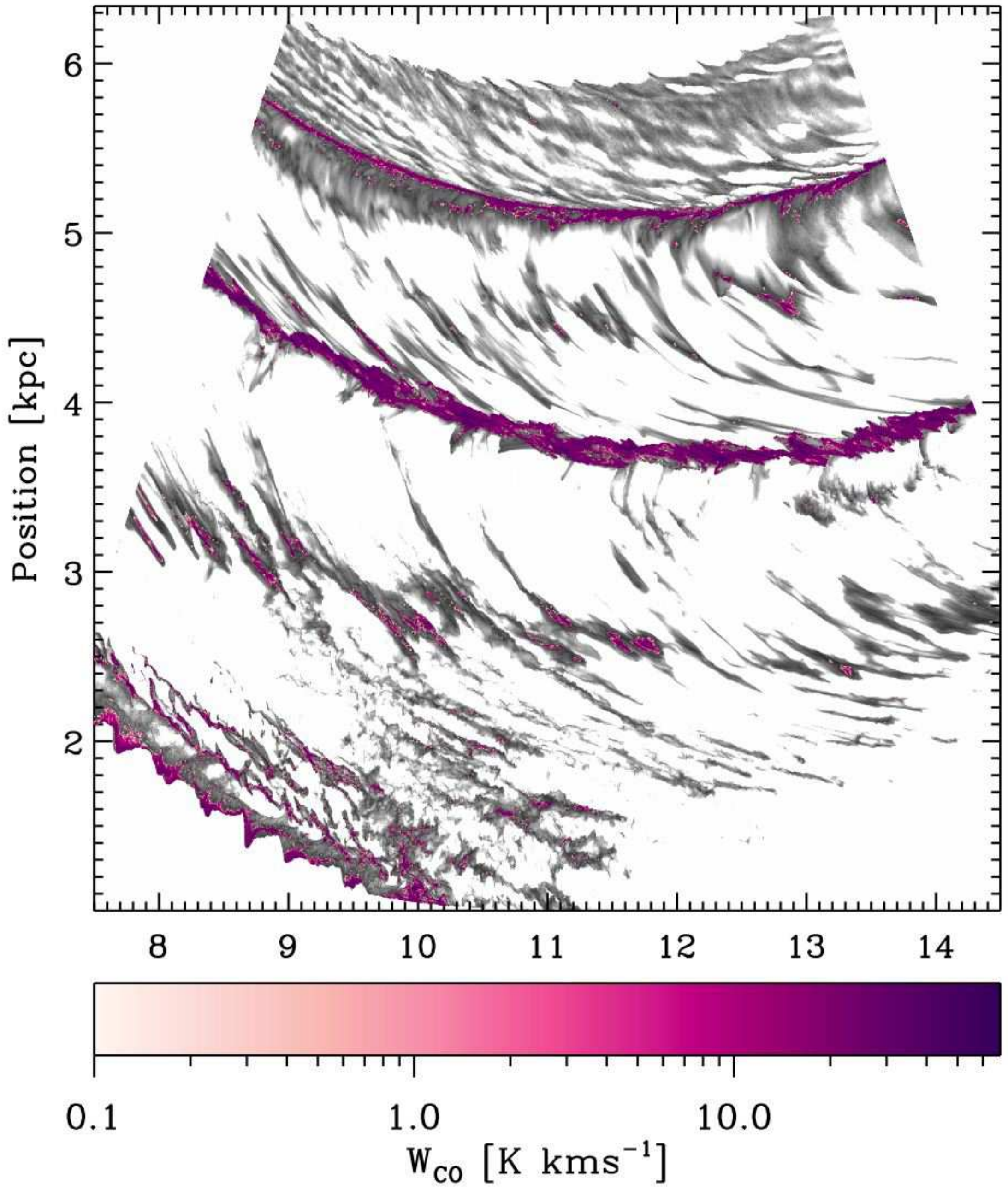
(Smith et al., 2014, MNRAS, 441, 1628)





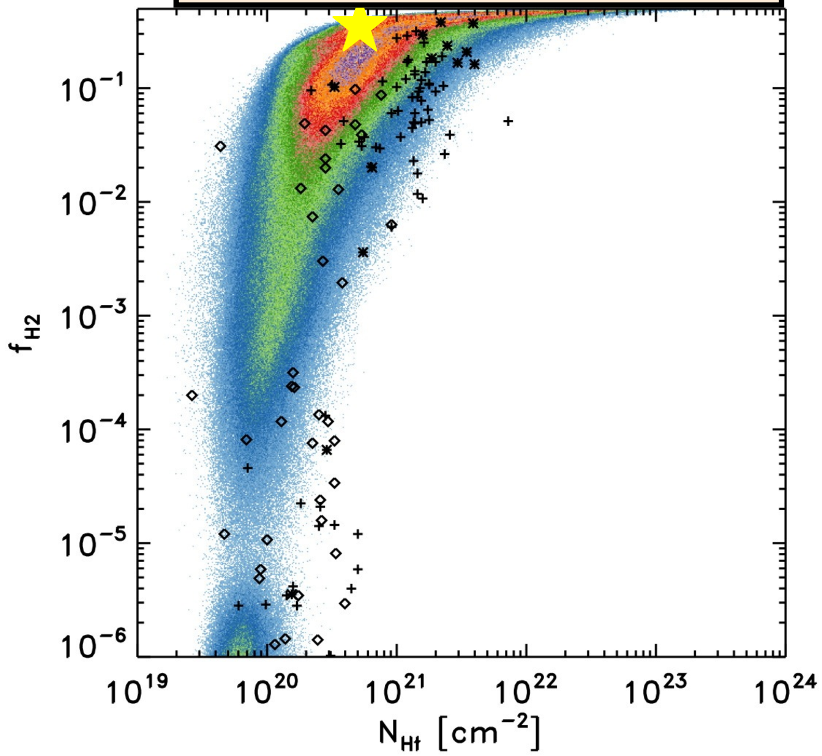


CO column density

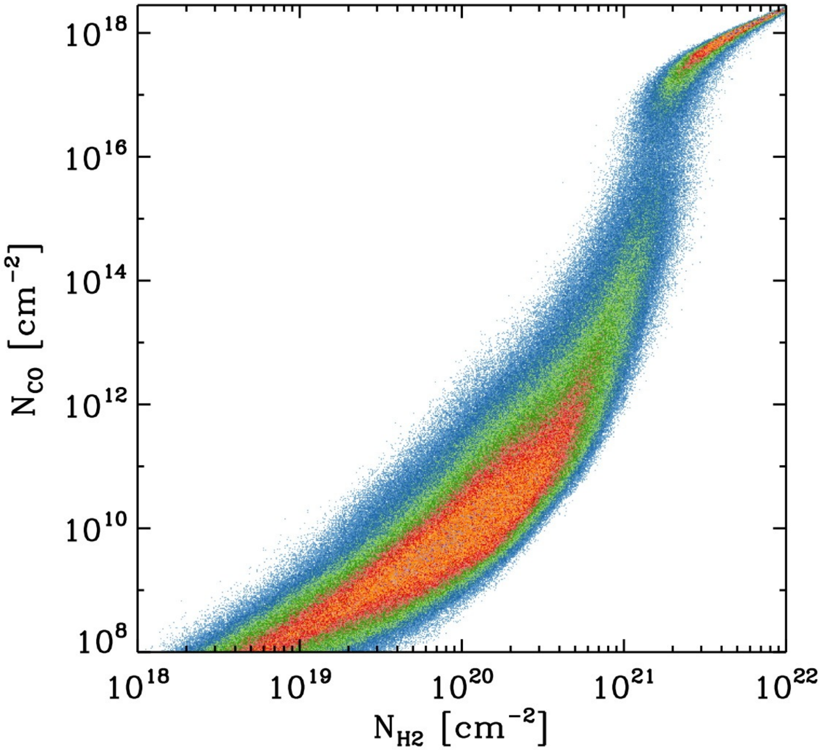


(Smith et al., 2014, MNRAS, 441, 1628)

H_2 fraction vs. column density N



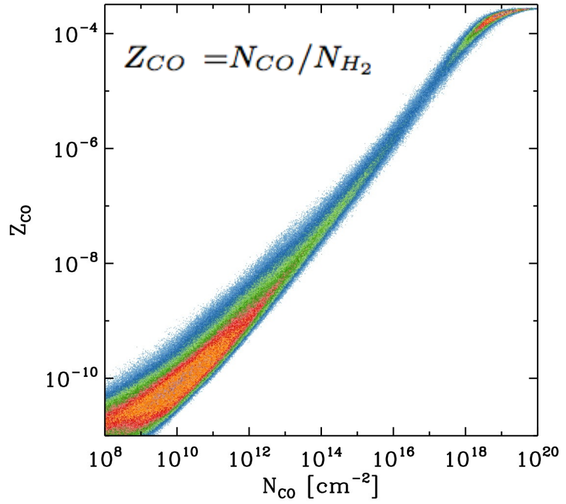
CO col. density vs. H_2 col. density



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

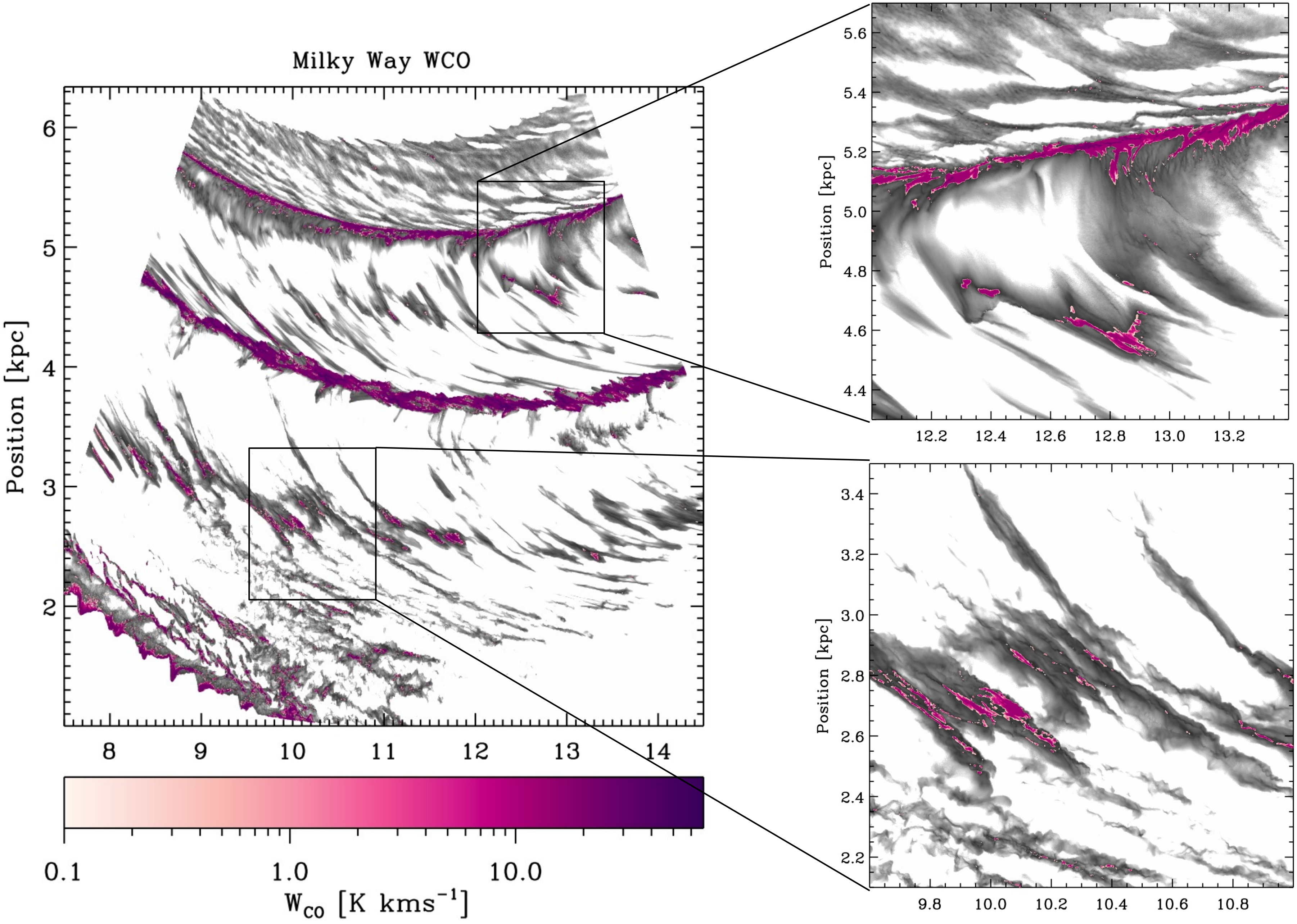
CO columns jump after $N_{H2} \sim 10^{21}$ cm^{-2}

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



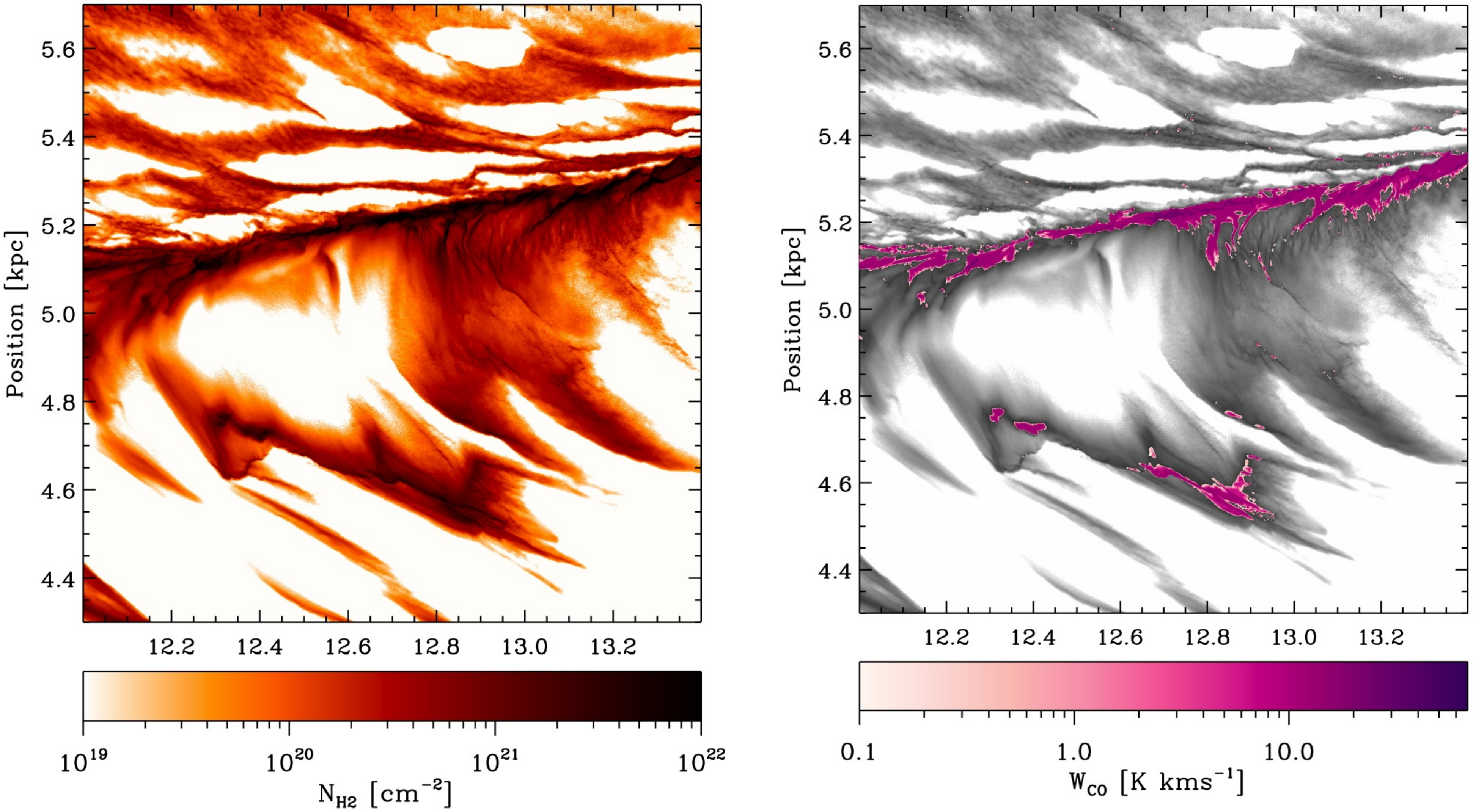
(Smith et al., 2014, MNRAS, 441, 1628)

details of CO emission



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

relation between CO and H_2



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

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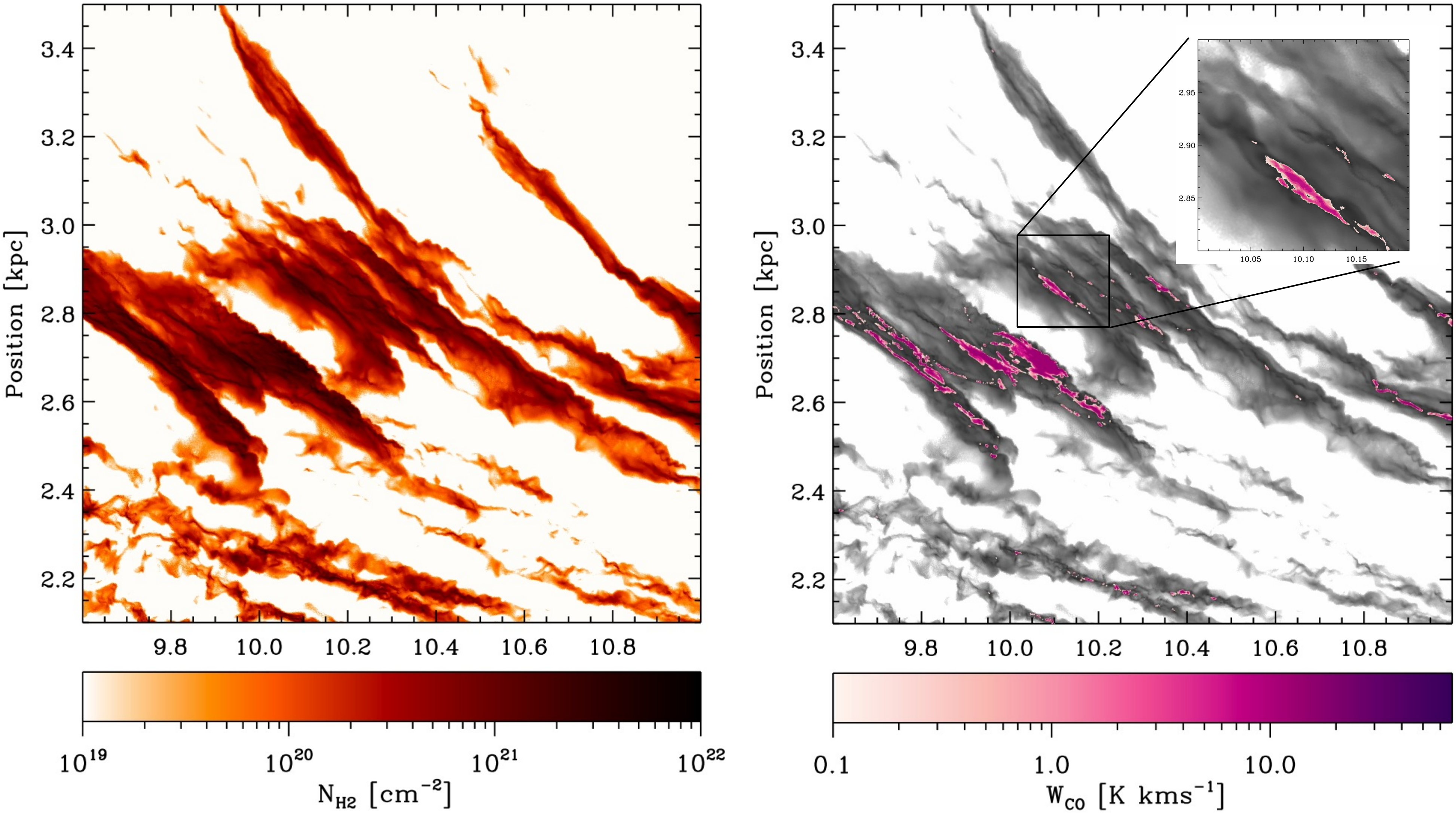
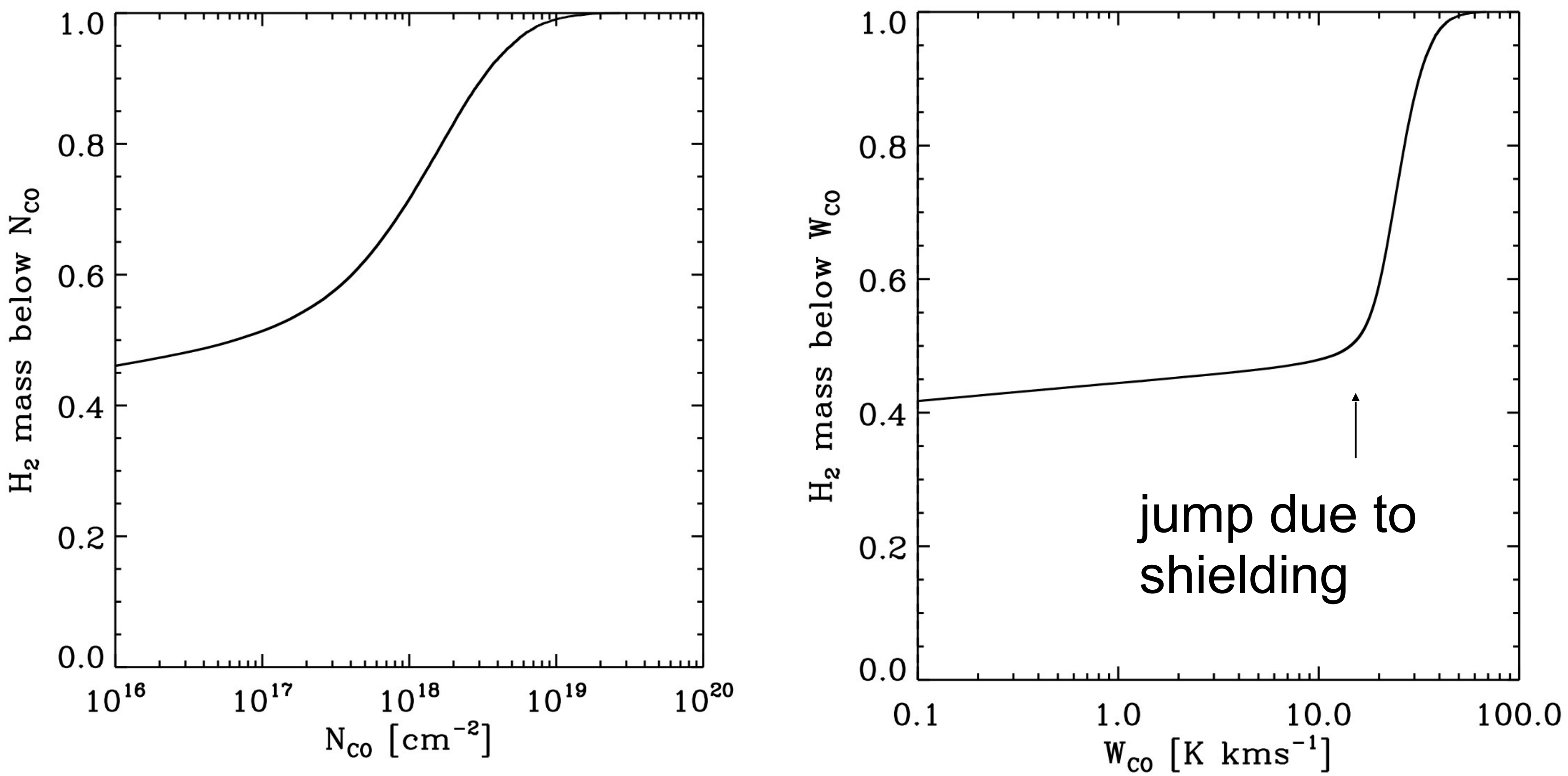


Filamentary molecular clouds in inter-arm regions are likely only the observable parts of much larger structures.

dark gas fraction



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

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

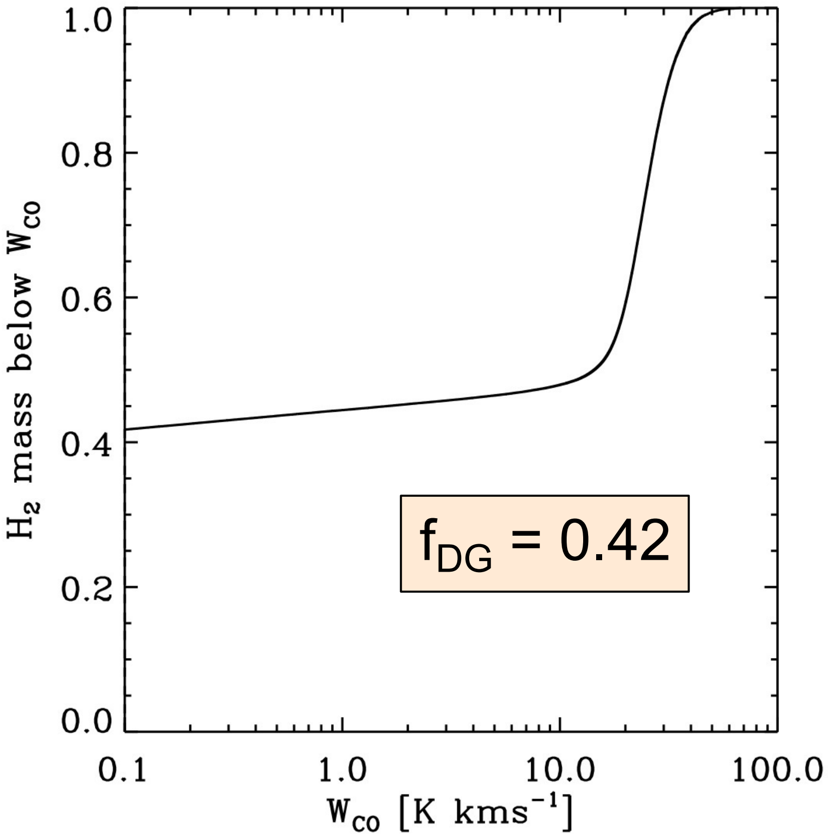
$f_{DG} = 0.42$ $X_{co}=2.2 \times 10^{20}$ cm^{-2}K^{-1}km^{-1}s

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

dark gas fraction

Observational estimates:

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



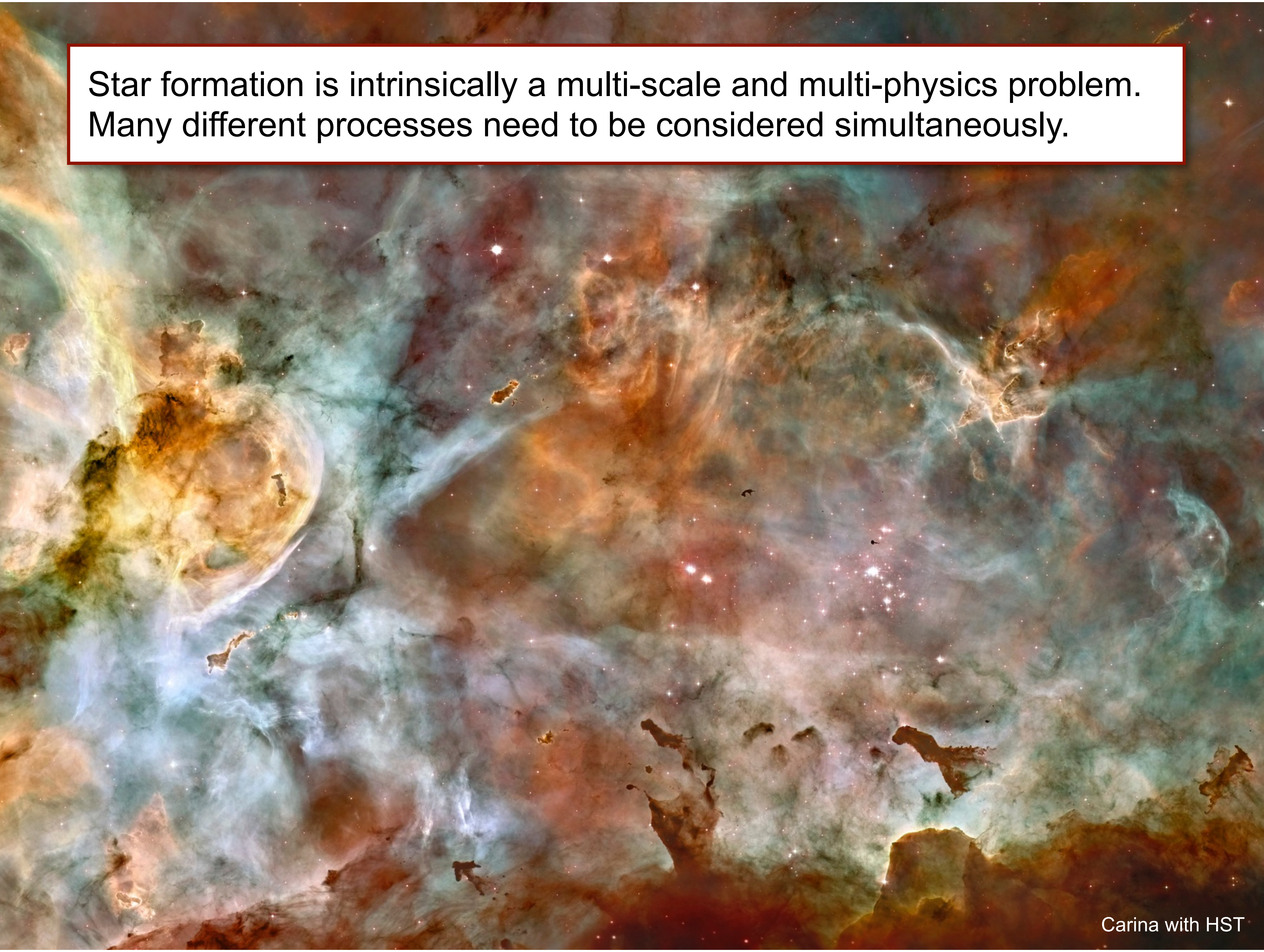
f_{DG} = 0.42

* dust methods have large uncertainties.

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

Carina with HST

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



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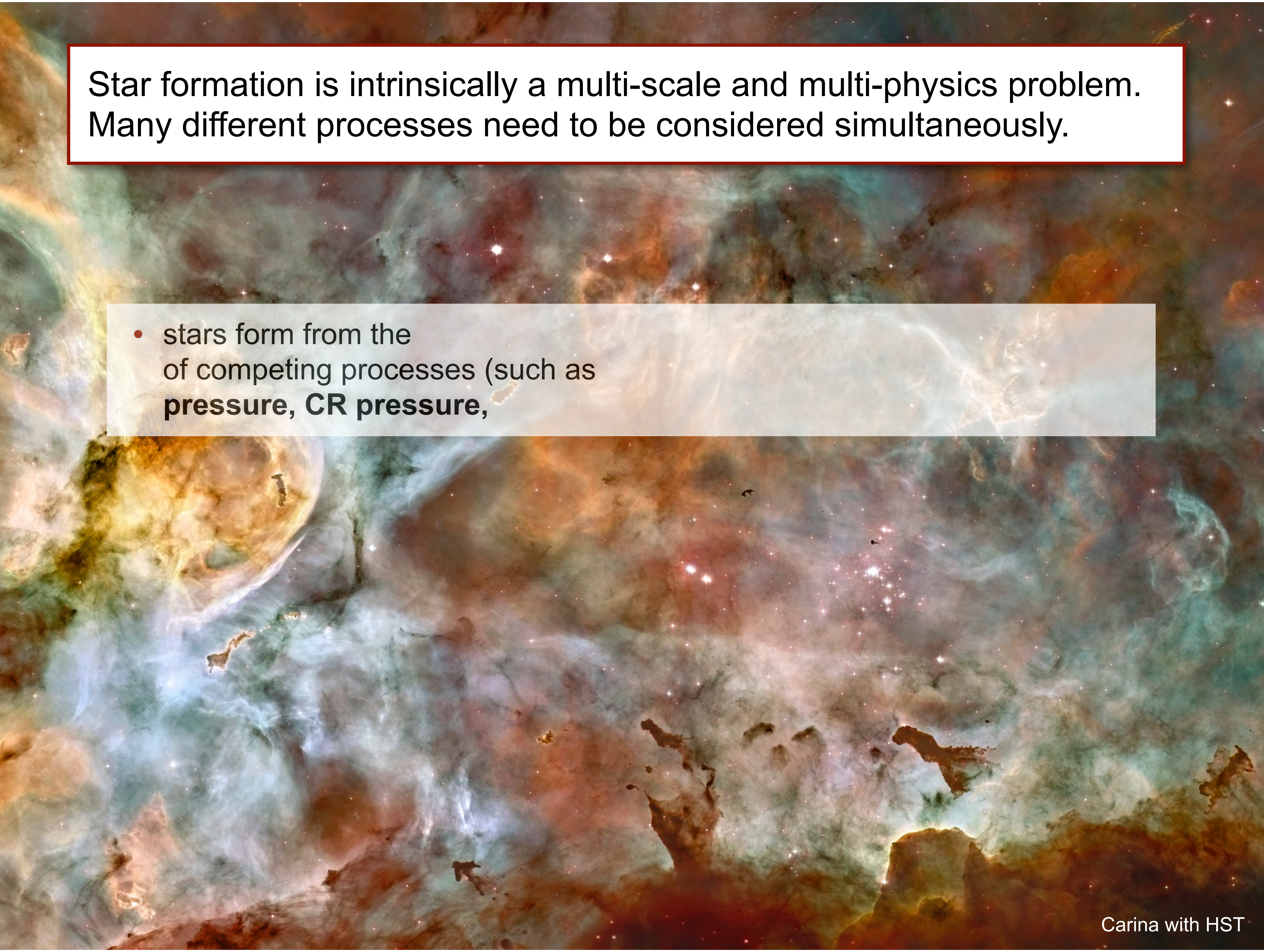

- stars form from the
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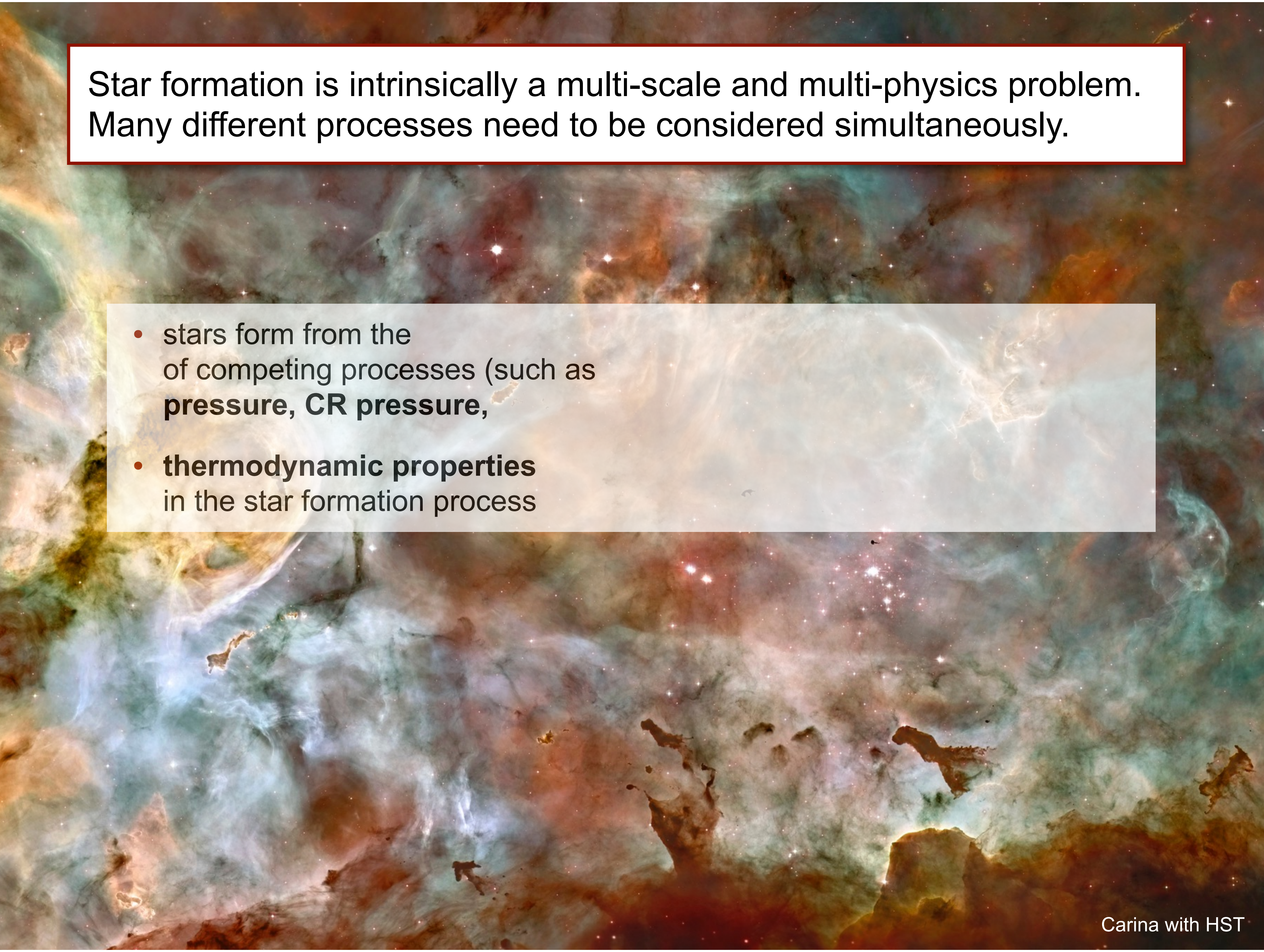
Carina with HST



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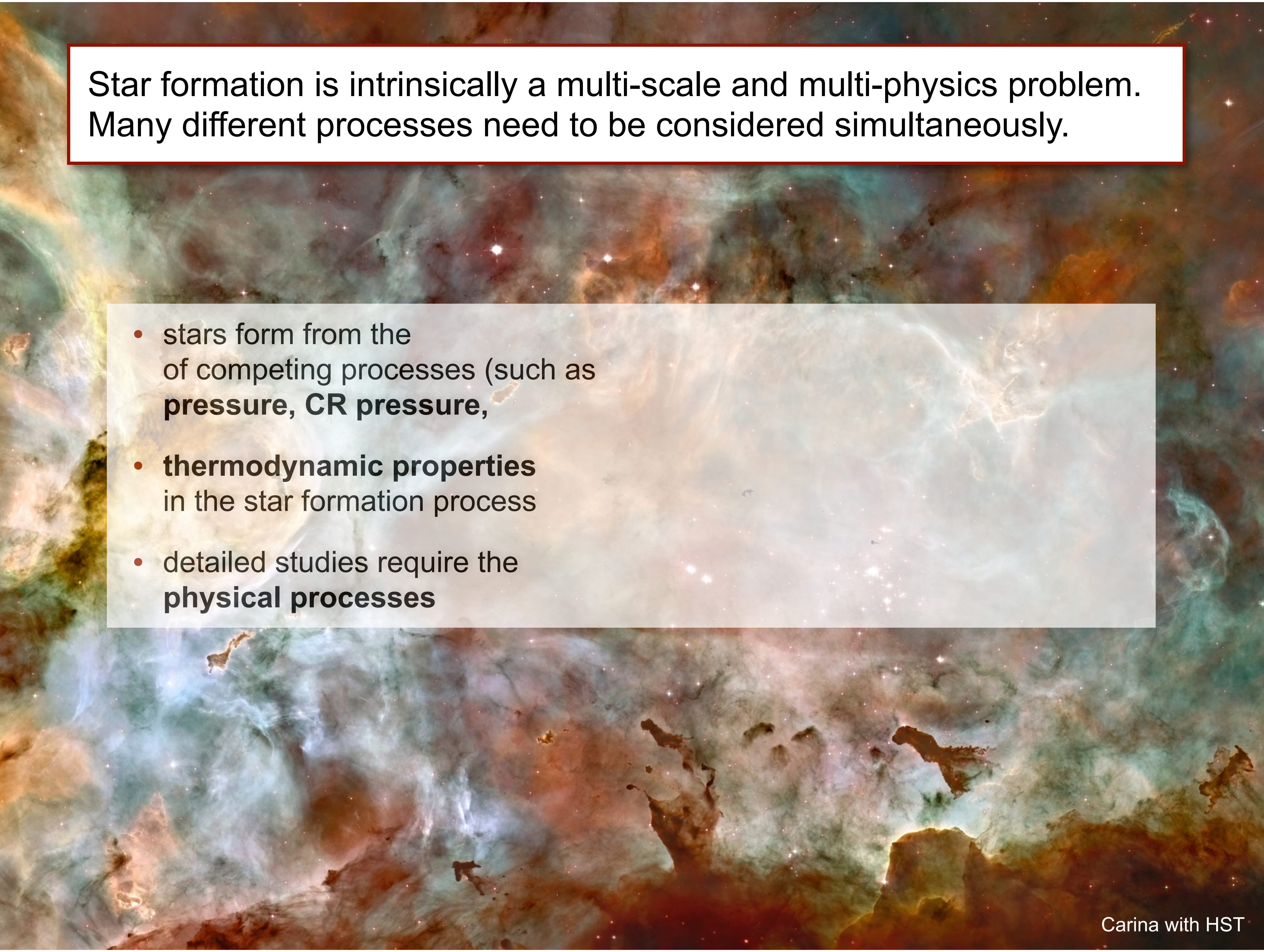

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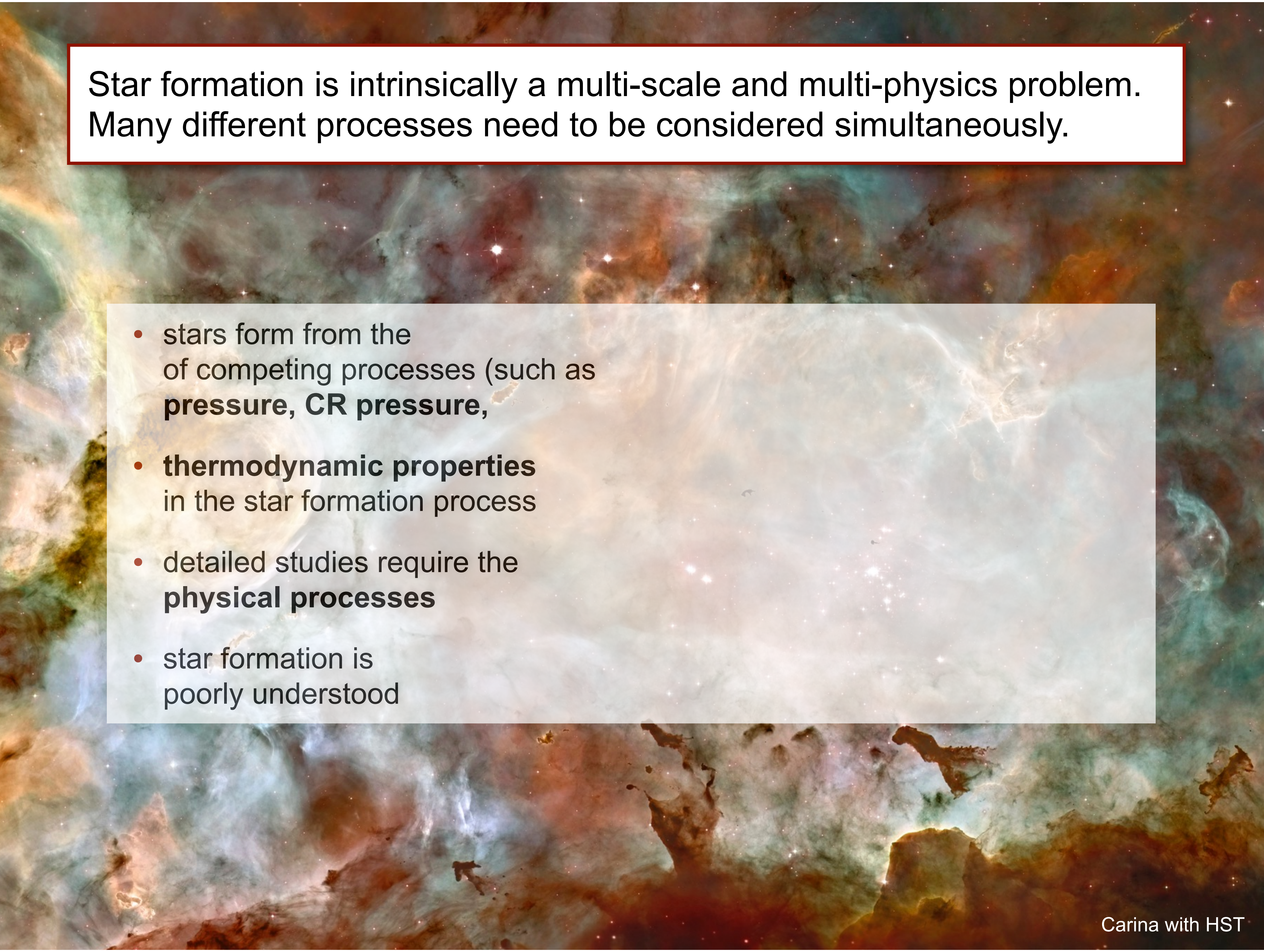

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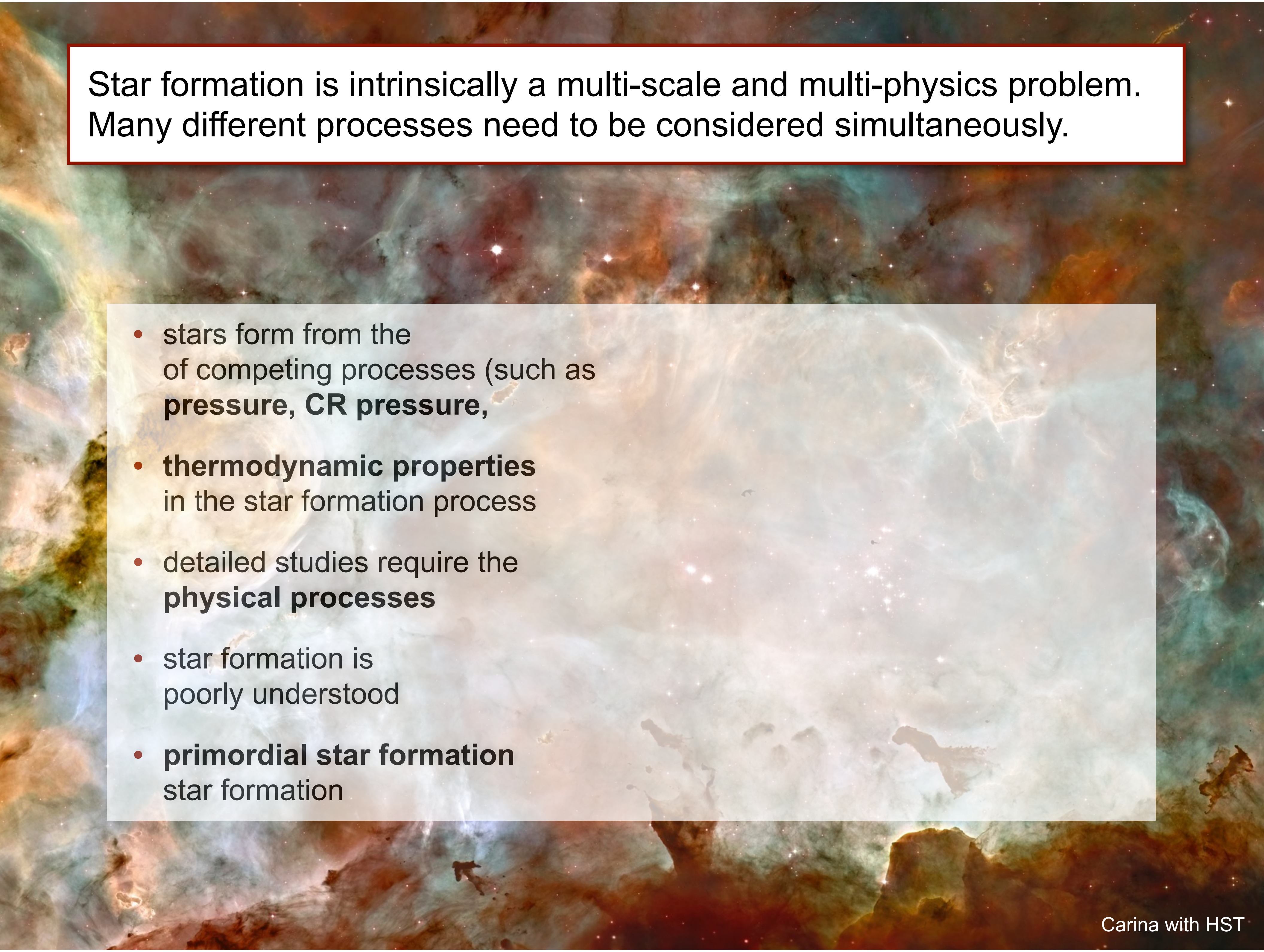
Carina with HST

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, CR pressure,**
- **thermodynamic properties** in the star formation process
- detailed studies require the **physical processes**
- star formation is poorly understood
- **primordial star formation** star formation



Carina with HST

Star formation is intrinsically a multi-scale and multi-physics problem.
It has close links to very diverse fields of modern astrophysics.

THANKS