



thanks to ...

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Agenda

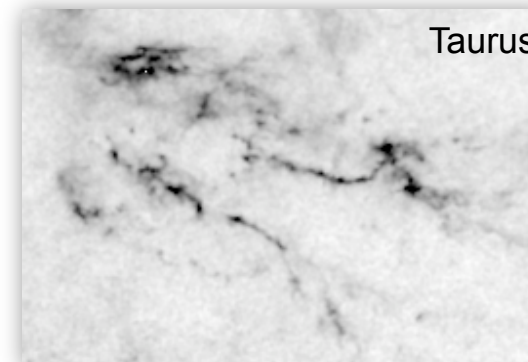
● some phenomenology

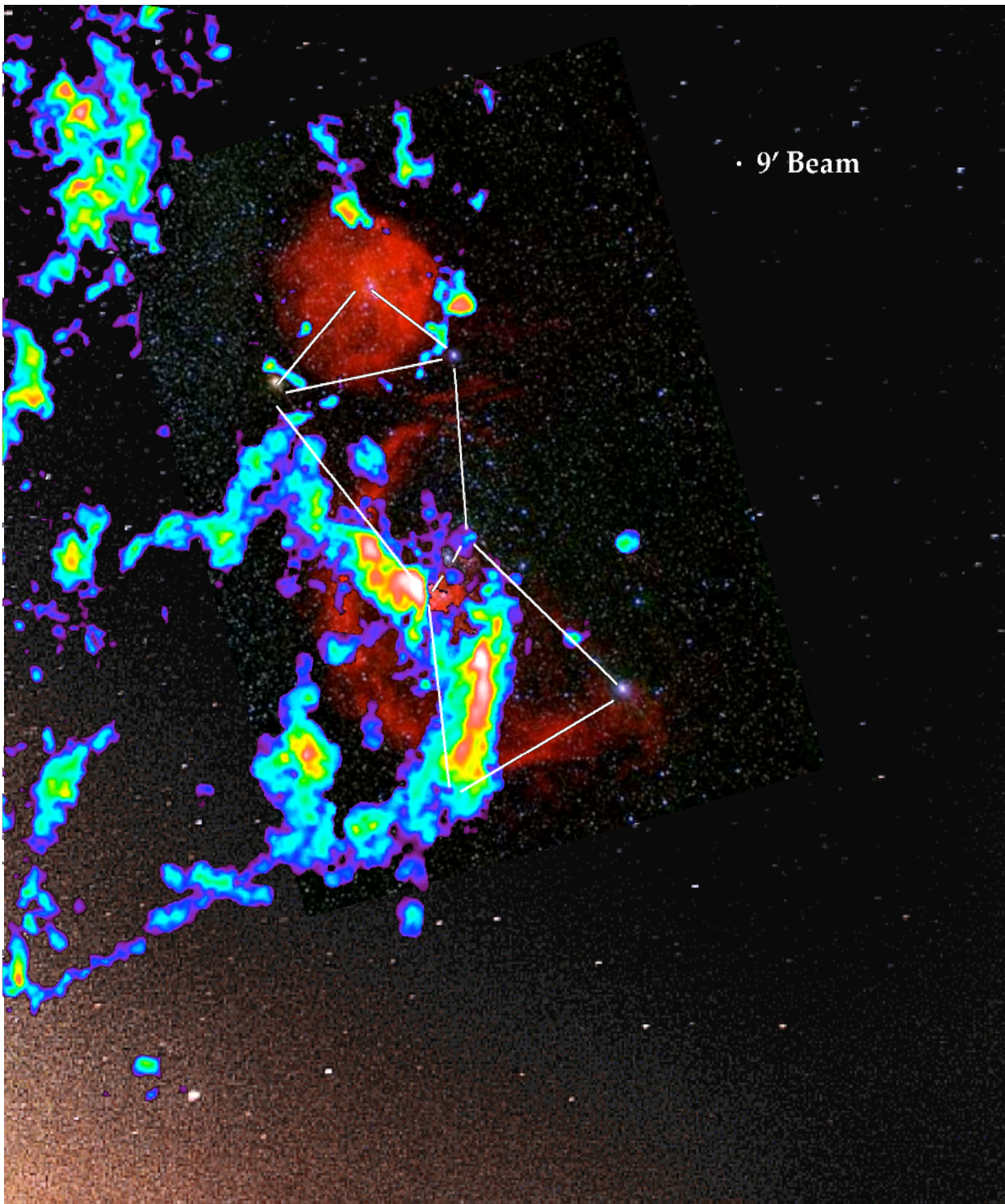
- what we know
- what we need to explain

● turbulence in the ISM

- some basic properties
- statistics of turbulence (solenoidal vs. dilatational modes)
- including more physics: time-dependent chemistry
----> formation of molecular clouds
- the first (strong) magnetic fields in the universe

● summary



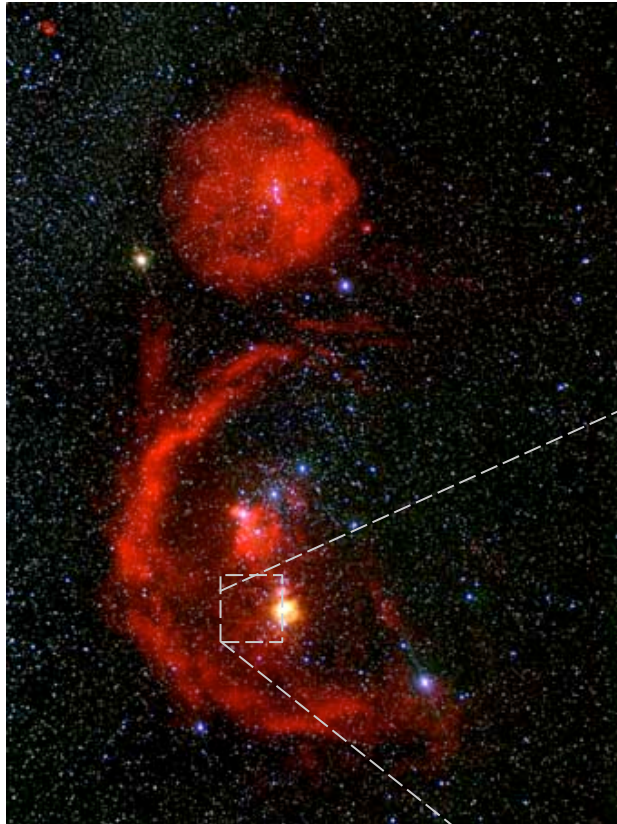


Star formation in Orion

We see

- *Stars* (in visible light)
- Atomic hydrogen (in $H\alpha$ -- red)
- Molecular hydrogen H_2 (radio emission -- color coded)

Local star forming region: The Trapezium Cluster in Orion



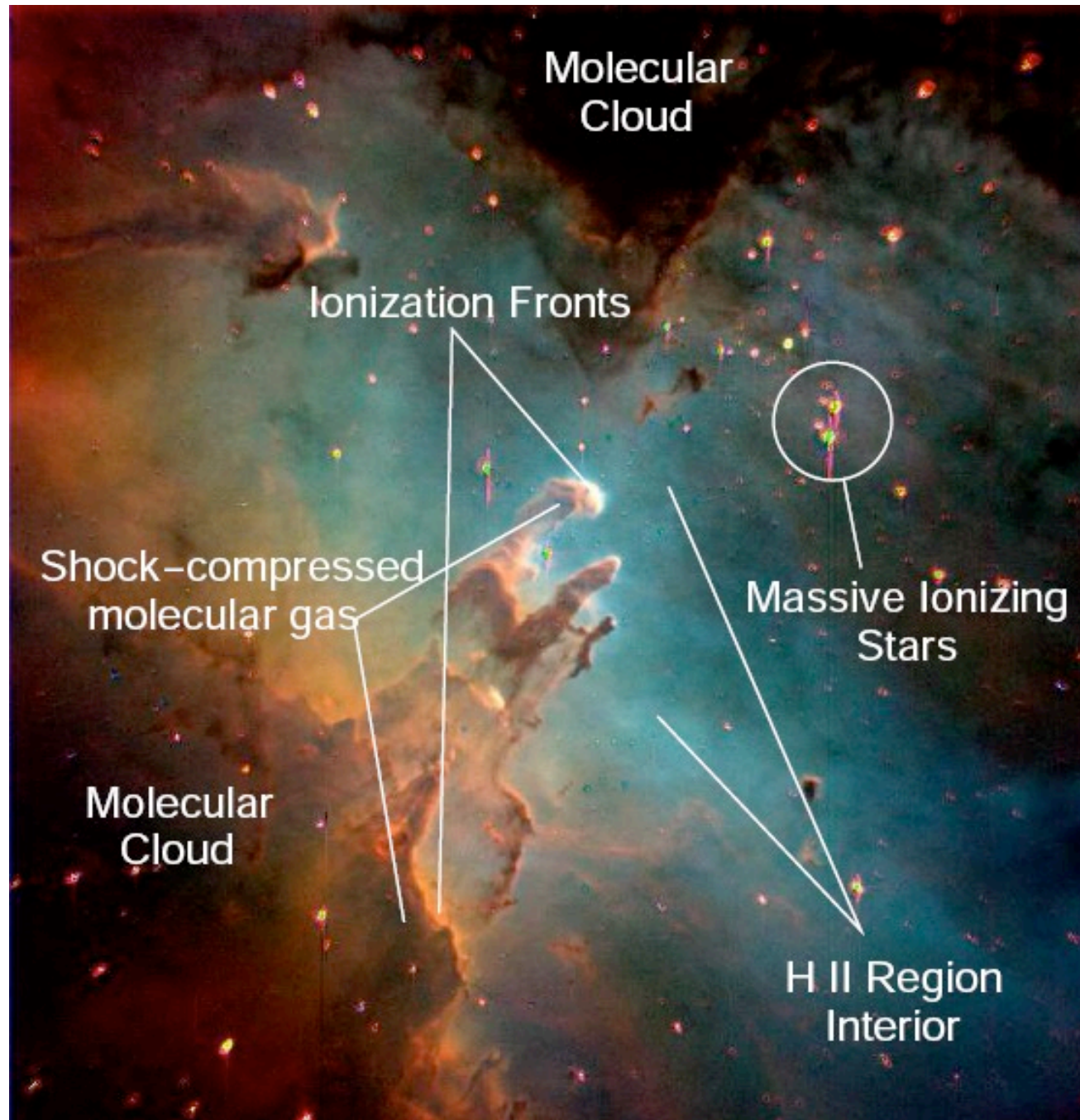
Orion molecular cloud

The Orion molecular cloud is the birth- place of several young embedded star clusters.

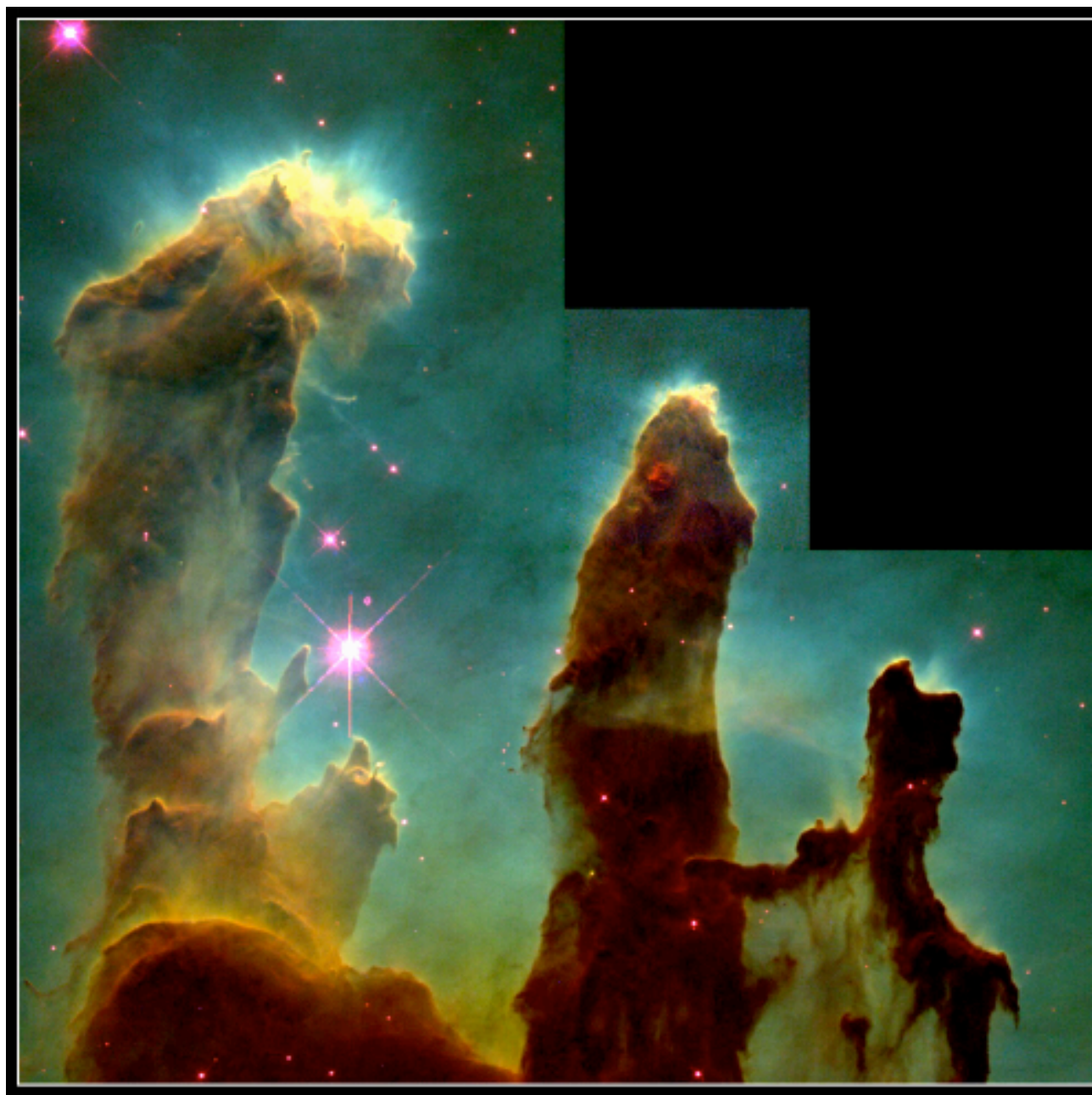
The Trapezium cluster is only visible in the IR and contains about 2000 newly born stars.



Trapezium cluster



alles in einem Bild



HST Aufnahme

Pillars of God (in Eagle Nebula): Formation of small groups of young stars in the tips of the columns of gas and dust

Ralf Klessen: San Diego, 15.06.2010



(
(

Infrared
observation



P
gr
of



Head of Column No.1 in Eagle Nebula (IR-View)
(VLT ANTU + ISAAC)

ESO PR Photo 57c/01 (20 December 2001)

© European Southern Observatory



IR observation with ESO-VLT

Pillars of God (in Eagle Nebula): Formation of small groups of young stars in the tips of the columns of gas and dust



Head of Column No.2 in Eagle Nebula (IR-View)
(VLT ANTU + ISAAC)

ESO PR Photo 37d/01 (20 December 2001)

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IR observation with ESO-VLT

Pillars of God (in Eagle Nebula): Formation of small groups of young stars in the tips of the columns of gas and dust

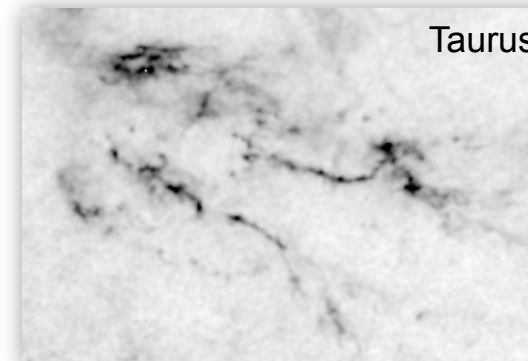


Interstellar Matter: ISM

Abundances, scaled to 1.000.000 H atoms

element atomic number abundance

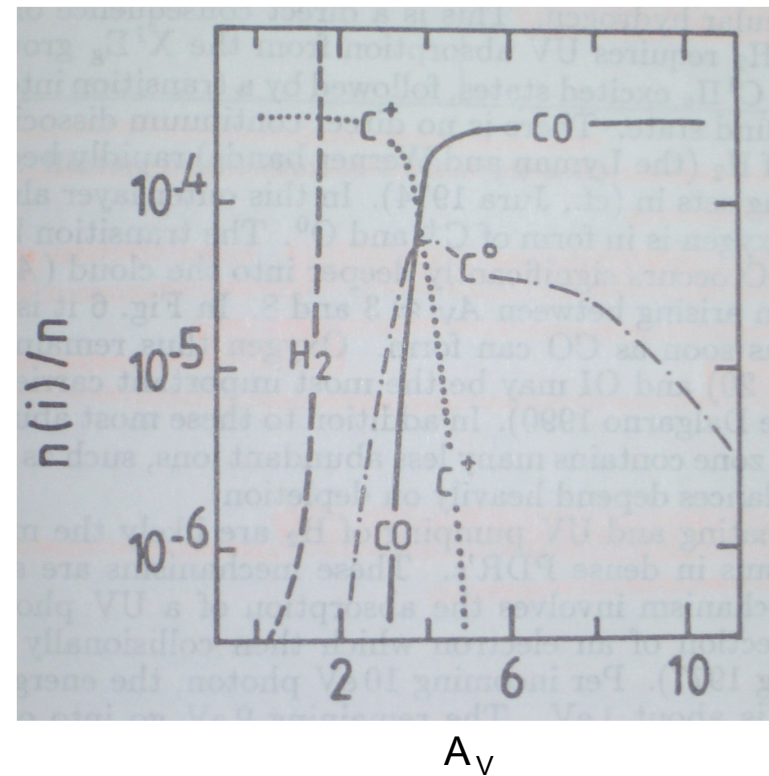
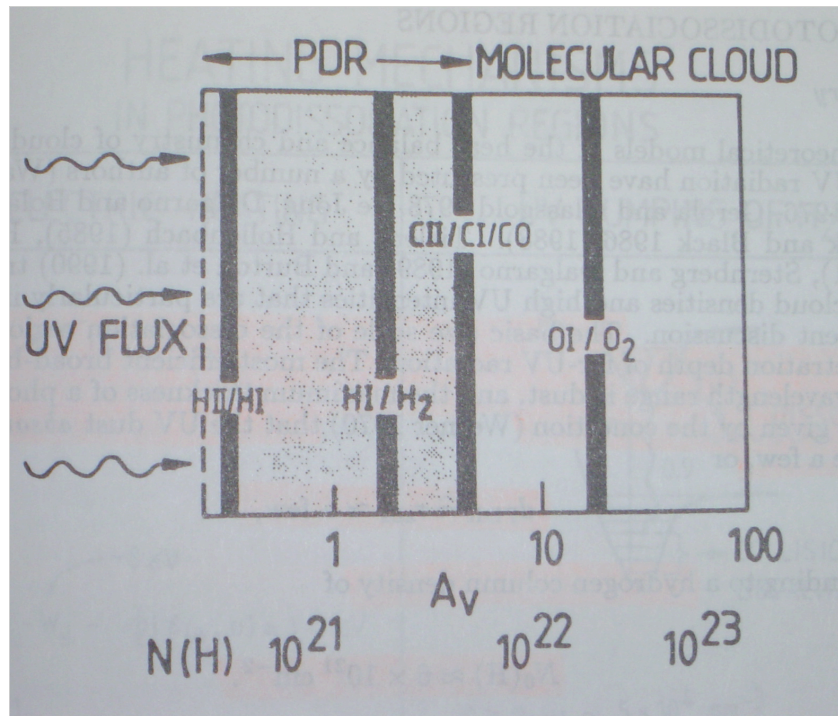
hydrogen	H	1	1.000.000
deuterium	${}_1\text{H}^2$	1	16
helium	He	2	68.000
carbon	C	6	420
nitrogen	N	7	90
oxygen	O	8	700
neon	Ne	10	100
sodium	Na	11	2
magnesium	Mg	12	40
aluminium	Al	13	3
silicium	Si	14	38
sulfur	S	16	20
calcium	Ca	20	2
iron	Fe	26	34
nickel	Ni	28	2



hydrogen is by far the most abundant element (more than 90% in number).



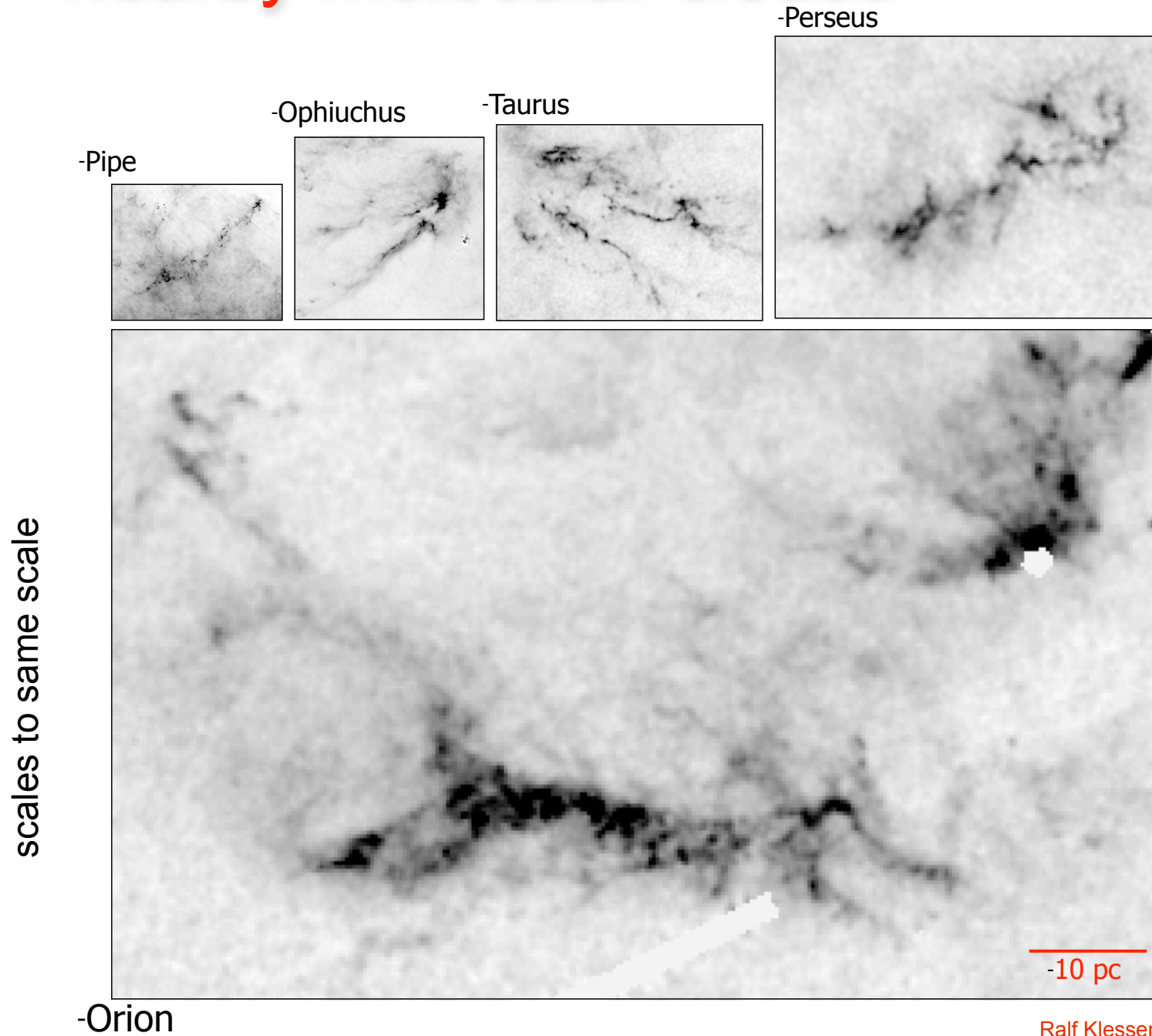
Phases of the ISM



A_V denotes the extinction, the attenuation of radiation due to absorption (mostly on dust grains)



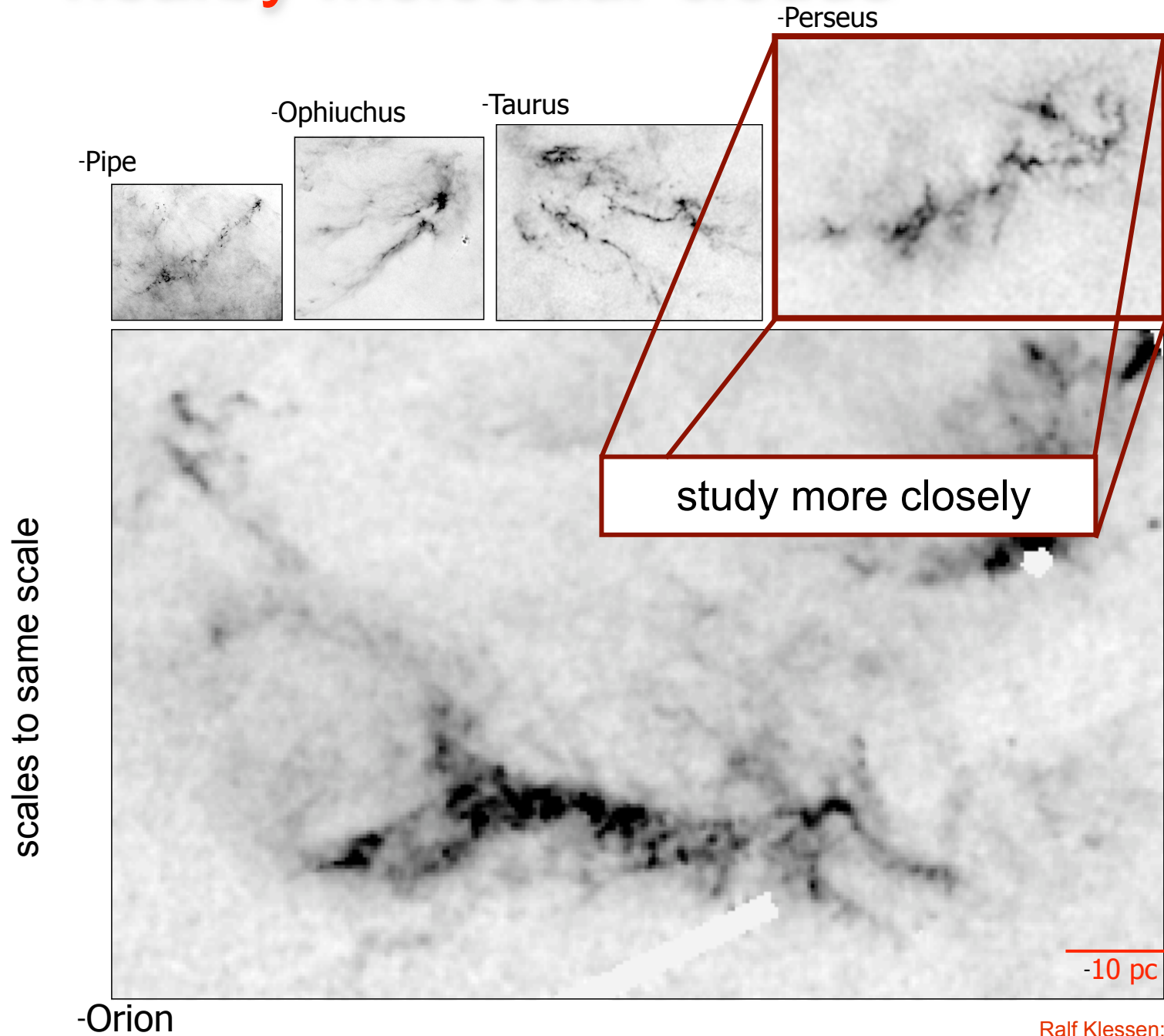
nearby molecular clouds



(from A. Goodman)



nearby molecular clouds



(from A. Goodman)

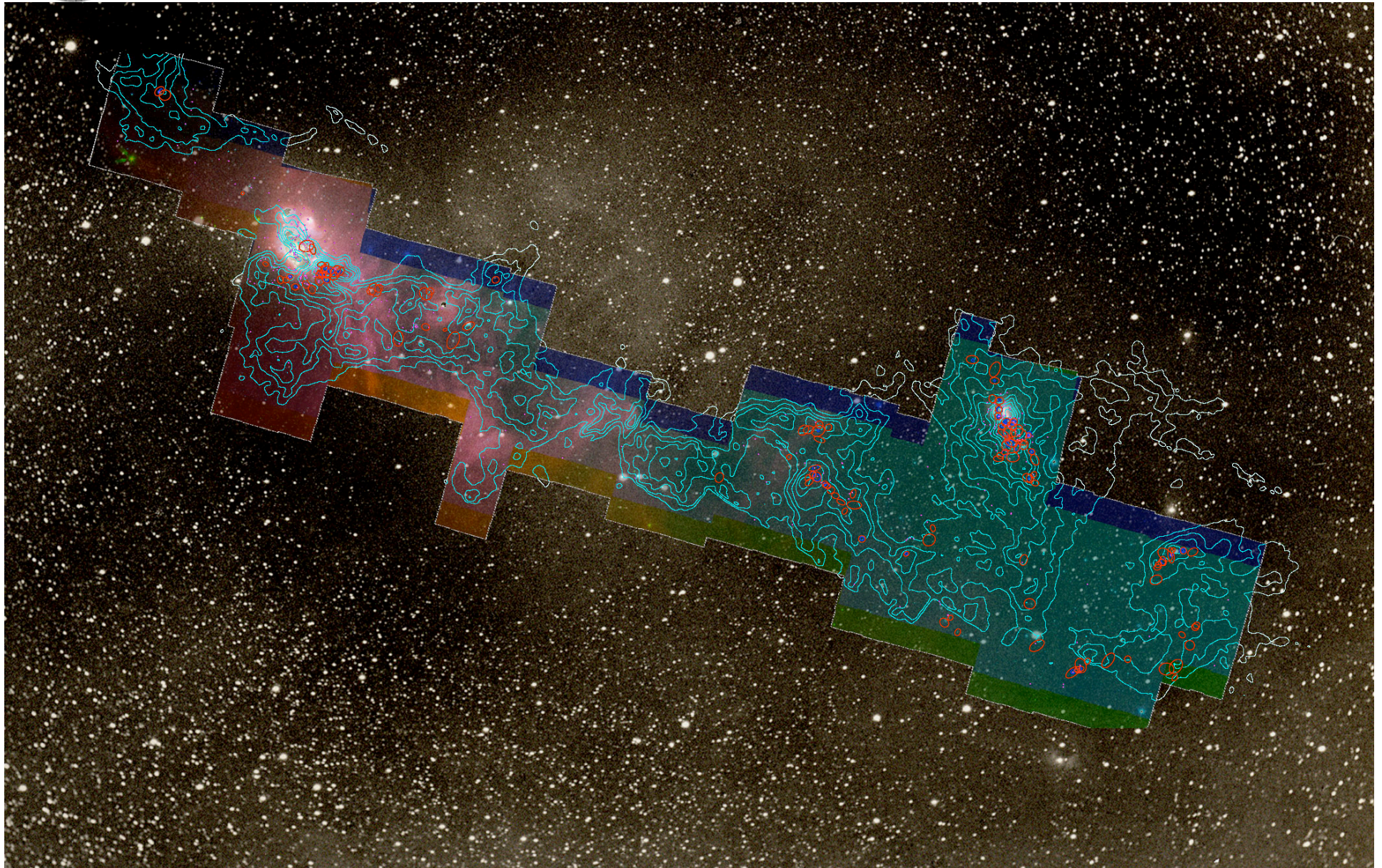
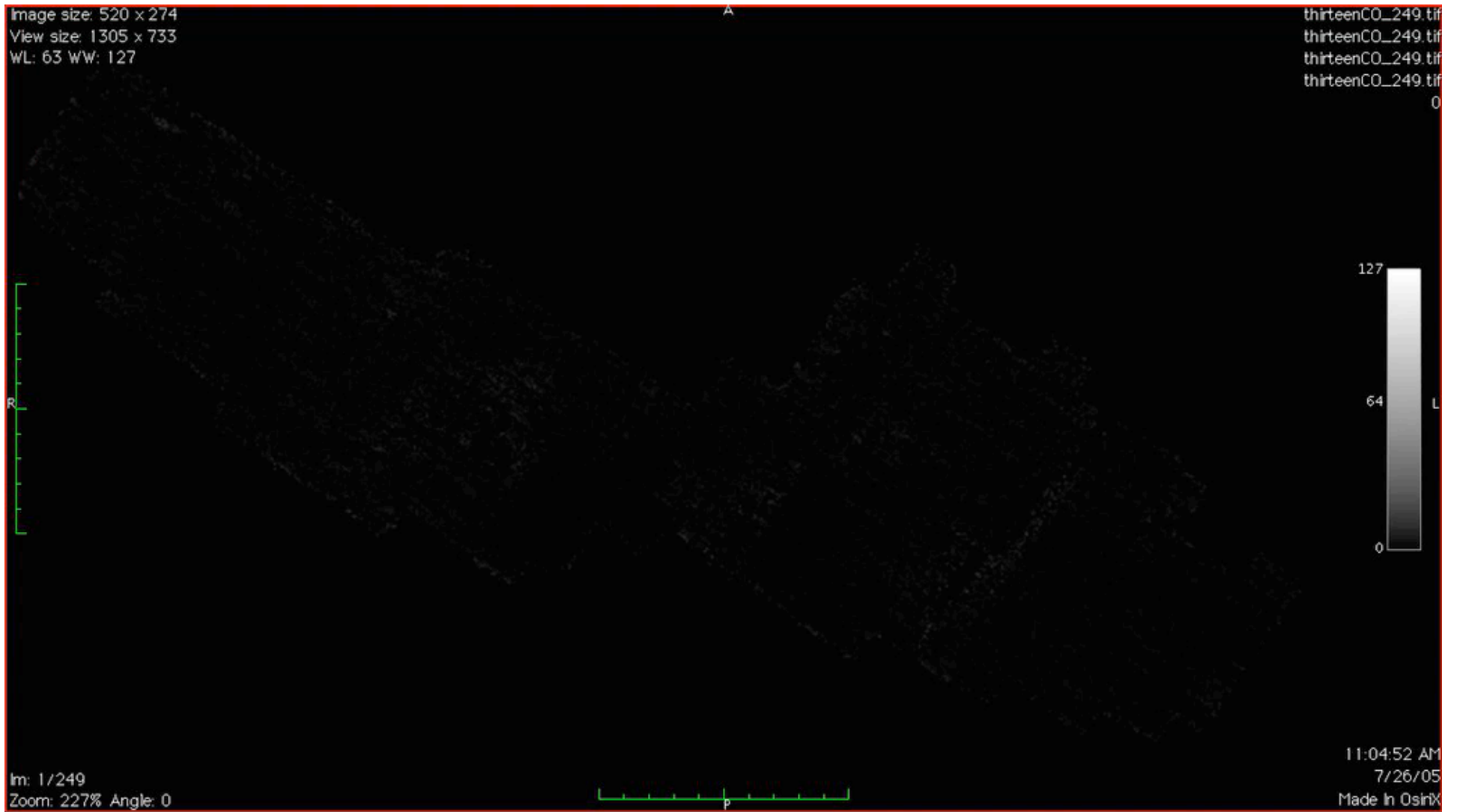


image from Alyssa Goodman: COMPLETE survey



velocity distribution in Perseus

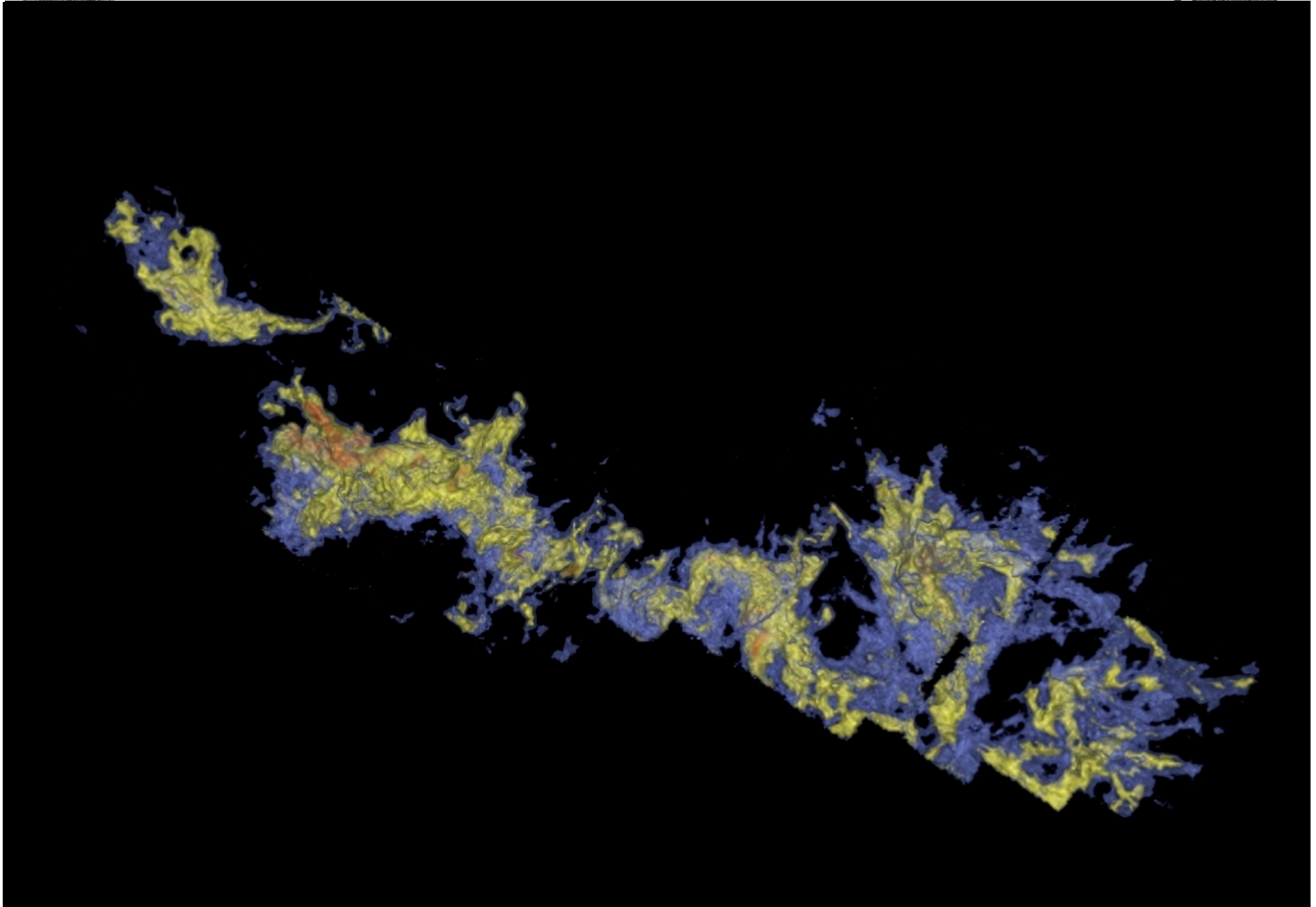
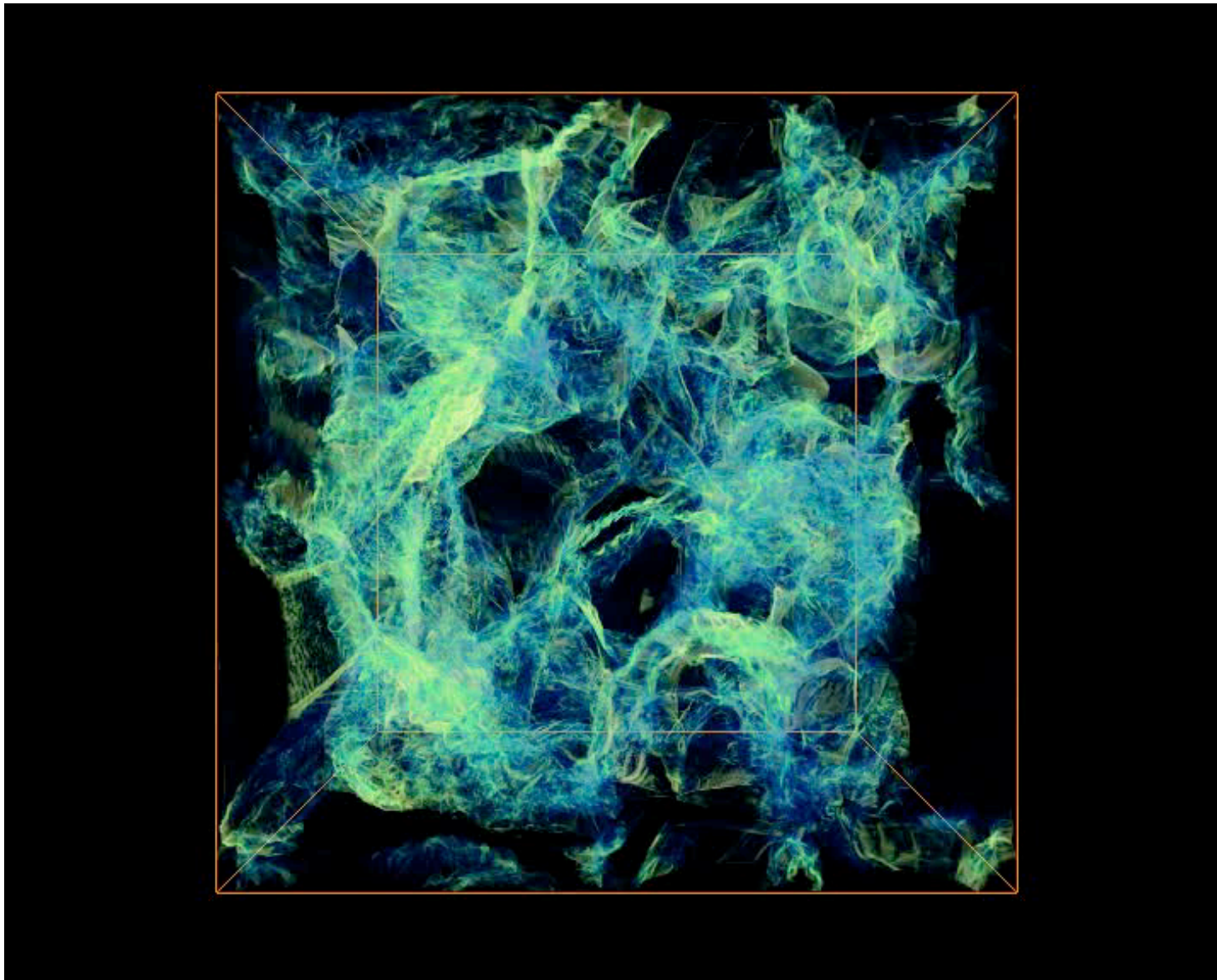


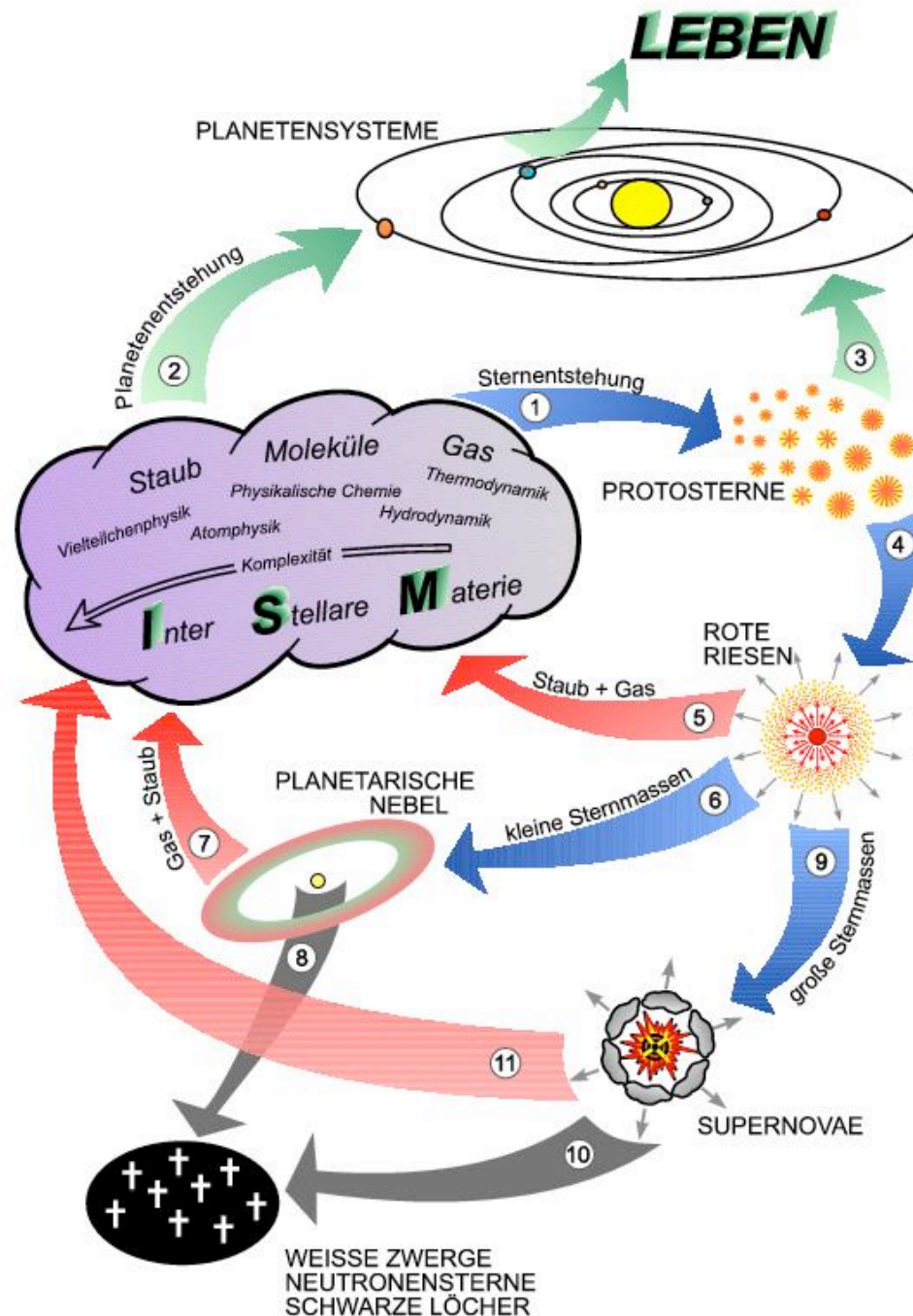
image from Alyssa Goodman: COMPLETE survey



(movie from Christoph Federrath)



what we want



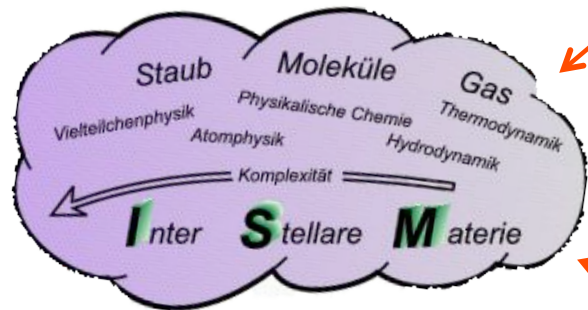
it is this complex matter cycle that we want to model

feedback loops on virtually all scales

multi-scale and multi-physics problem



What do we need to study ISM?



magneto-hydrodynamics

(multi-phase, non-ideal MHD, turbulence)

chemistry (gas + dust, heating + cooling)

radiation (continuum + lines)

stellar dynamics

(collisional: star clusters, collisionless: galaxies, DM)

stellar evolution

(feedback: radiation, winds, SN)

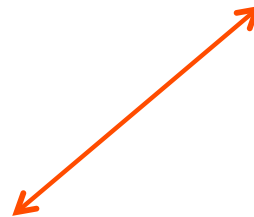
+ laboratory work

(reaction rates, cross sections, dust coagulation properties, etc.)



What do we need to study ISM?

- massive parallel codes
- particle-based: SPH with improved algorithms (XSPH with turb. subgrid model, GPM, particle splitting, MHD-SPH?)
- grid-based: AMR (FLASH, ENZO, RAMSES, Athena, Nirvana3, etc), subgrid-scale models (FEARLESS)
- BGK methods



magneto-hydrodynamics

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+ **laboratory work**

(reaction rates, cross sections, dust coagulation properties, etc.)



What do we need to study ISM?

- ever increasing chemical networks
- working reduced networks for time-dependent chemistry in combination with hydrodynamics
- improved data on reaction rates (laboratory + quantum mechanical calculations)



magneto-hydrodynamics

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stellar evolution

(feedback: radiation, winds, SN)

+ **laboratory work**

(reaction rates, cross sections, dust coagulation properties, etc.)



What do we need to study ISM?

- continuum vs. lines
- Monte Carlo, characteristics
- approximative methods
- combine with hydro



magneto-hydrodynamics

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stellar evolution

(feedback: radiation, winds, SN)

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(reaction rates, cross sections, dust coagulation properties, etc.)



What do we need to study ISM?

- statistics: number of stars (collisional: 10^6 , collisionless: 10^{10})
- transition from gas to stars
- binary orbits
- long-term integration



magneto-hydrodynamics

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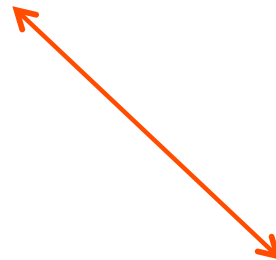
+ **laboratory work**

(reaction rates, cross sections, dust coagulation properties, etc.)



What do we need to study ISM?

- very early phases (pre main sequence tracks)
- massive stars at late phases
- role of rotation
- primordial star formation



magneto-hydrodynamics

(multi-phase, non-ideal MHD, turbulence)

chemistry (gas + dust, heating + cooling)

radiation (continuum + lines)

stellar dynamics

(collisional: star clusters, collisionless: galaxies, DM)

stellar evolution

(feedback: radiation, winds, SN)

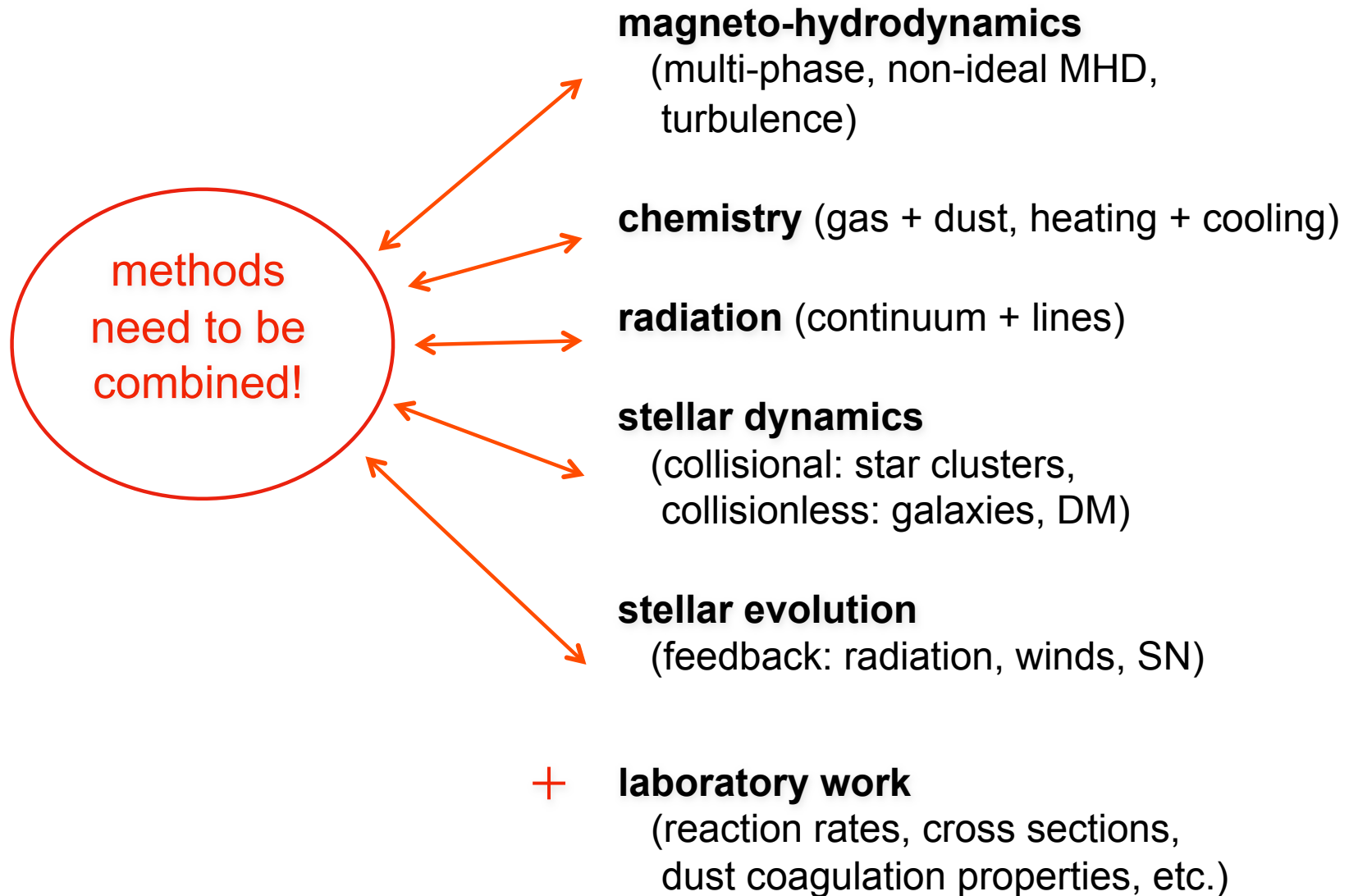
+

laboratory work

(reaction rates, cross sections, dust coagulation properties, etc.)



What do we need to study ISM?





challenges

- Problem of star formation is very complex. It involves many scales (10^7 in length, and 10^{20} in density) and many physical processes → NO analytic solution
→ NUMERICAL APPROACH
- BUT, we need to...
 - solve the MHD equations in 3 dimensions
 - solve Poisson's equation (self-gravity)
 - follow the full turbulent cascade (from galactic scales to stellar surface)
 - follow chemical evolution (time-dependent chemical network)
 - include heating / cooling processes (internal degrees of freedom)
 - treat radiation transfer



approach

- Simplify!
Divide problem into little bits and pieces....
- **GRAVOTURBULENT CLOUD FRAGMENTATION**
- We try to...
 - solve the HD equations in 3 dimensions
 - solve Poisson's equation (self-gravity)
 - include a (humble) approach to supersonic turbulence
 - include simple chemical network & tabulated cooling functions
 - follow collapse: include "sink particles"
(this will "handle" our subgrid-scale physics)



turbulence



Properties of turbulence

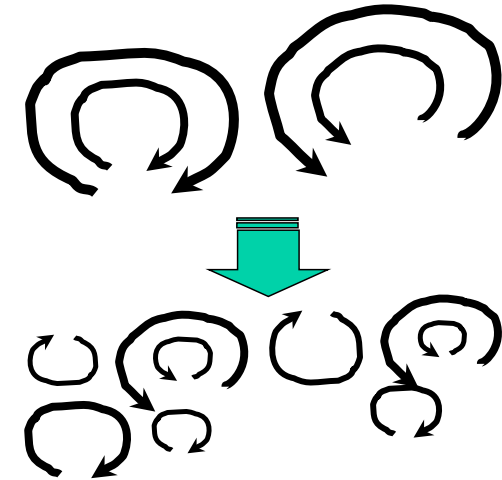
- laminar flows turn *turbulent* at *high Reynolds* numbers

$$\text{Re} = \frac{\text{advection}}{\text{dissipation}} = \frac{VL}{\nu}$$

V = typical velocity on scale L , ν = viscosity, $\text{Re} > 1000$

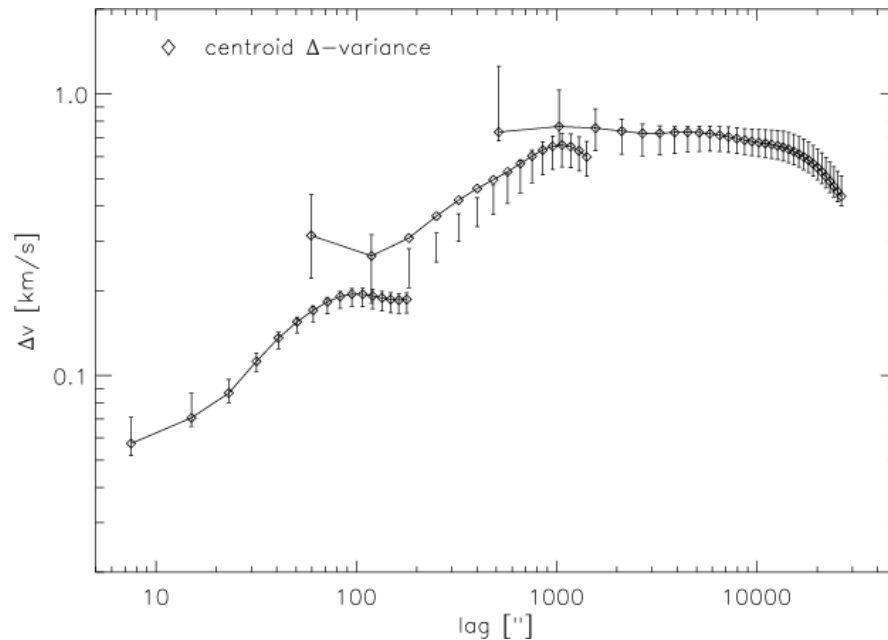
- *vortex stretching* --> turbulence is *intrinsically anisotropic* (only on large scales you *may* get homogeneity & isotropy in a statistical sense; see Landau & Lifschitz, Chandrasekhar, Taylor, etc.)

(ISM turbulence: shocks & B-field cause additional inhomogeneity)





what drives turbulence?



Polaris flare (from Ossenkopf & Mac Low 2002)

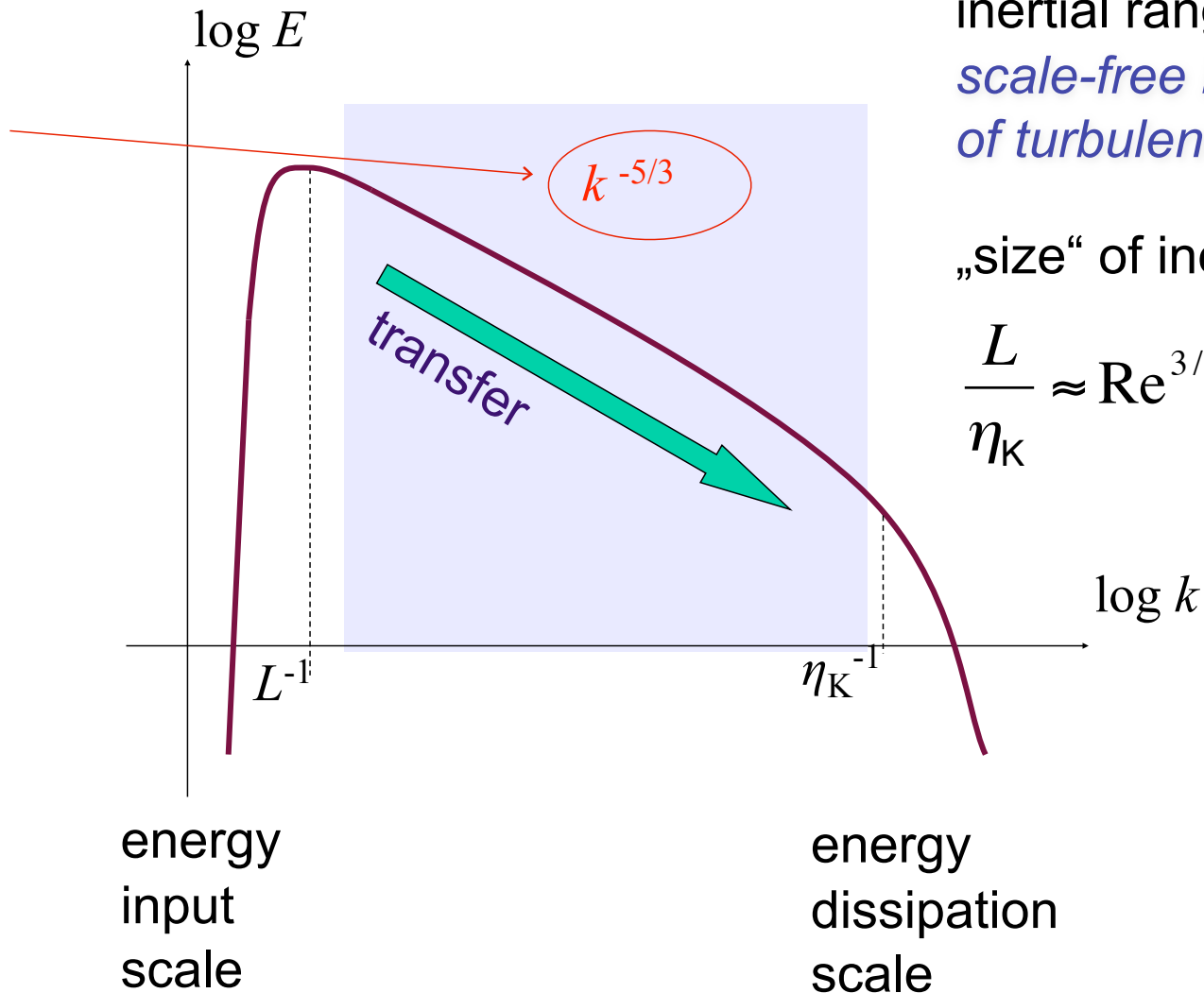
● turbulence characteristics

- molecular cloud turbulence seems to be dominated by large-scale models
- consistent with external driving
- convergent flows?
→ the same process that creates the cloud supplies internal turbulence ...
- alternative mechanisms:
 - gravity (spiral shocks), supernovae, HII regions?
 - internal sources: jets, outflows?



Turbulent cascade

Kolmogorov (1941) theory
incompressible turbulence



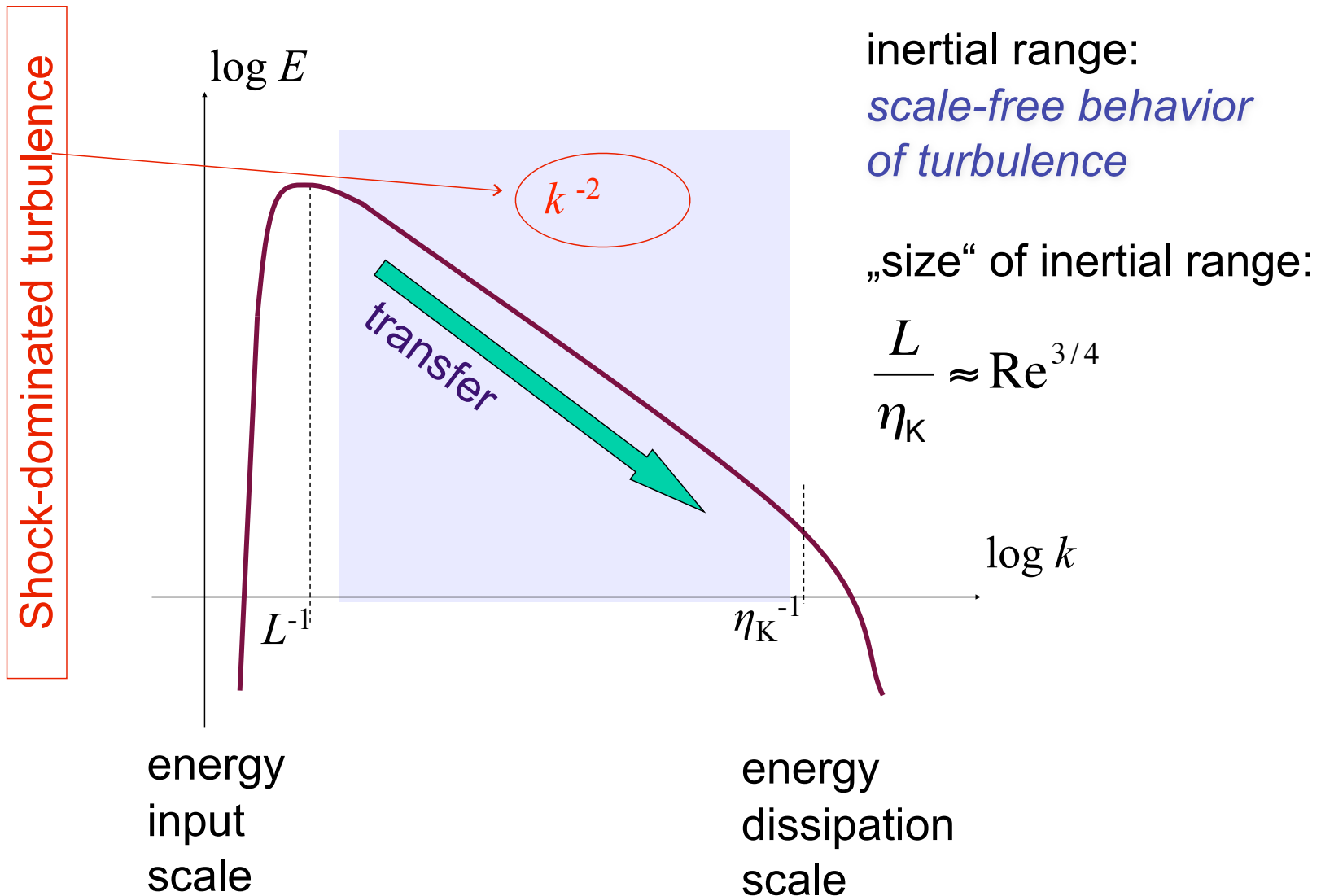
inertial range:
*scale-free behavior
of turbulence*

„size“ of inertial range:

$$\frac{L}{\eta_K} \approx \text{Re}^{3/4}$$

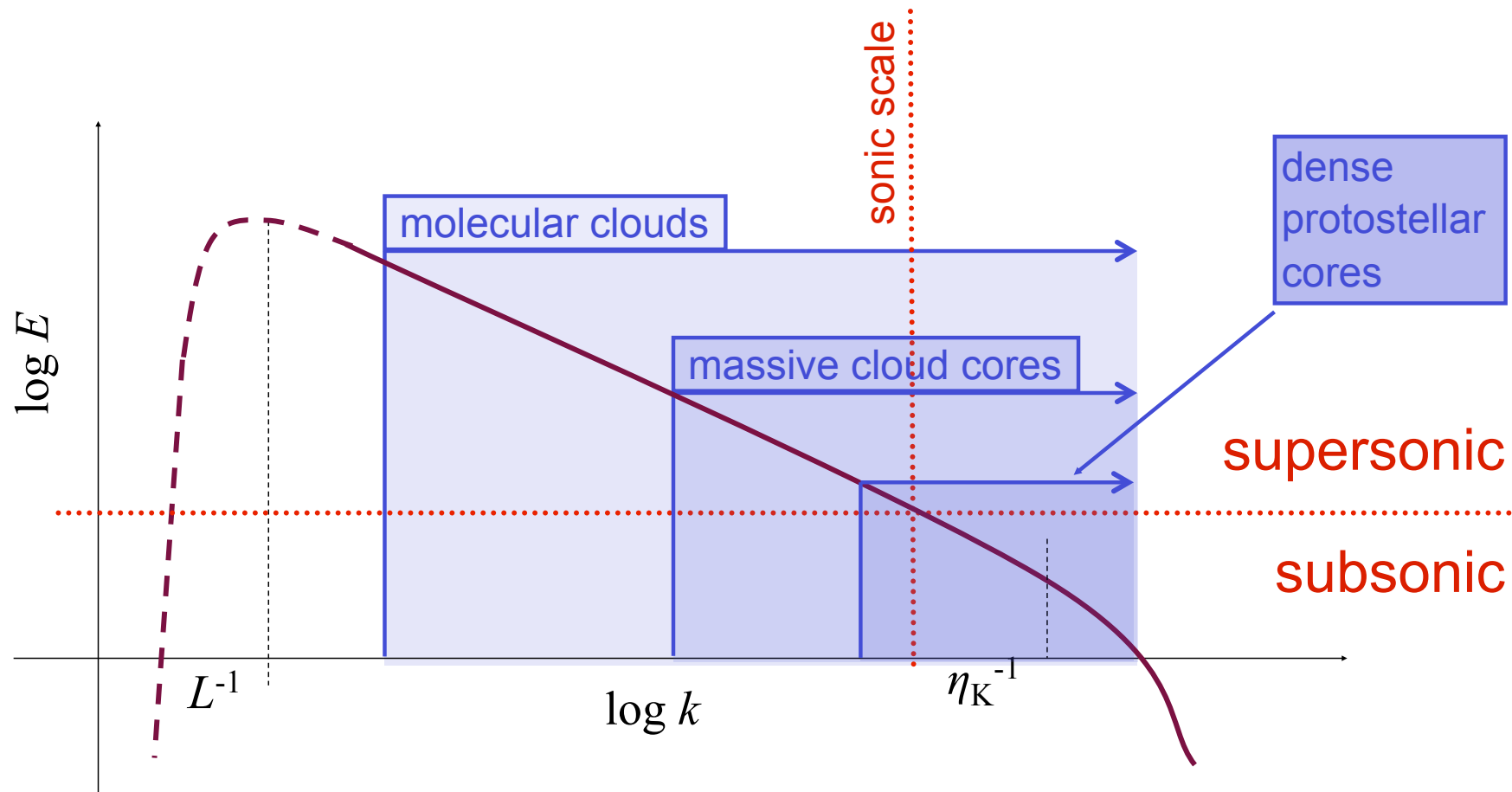


Turbulent cascade





Turbulent cascade in ISM



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

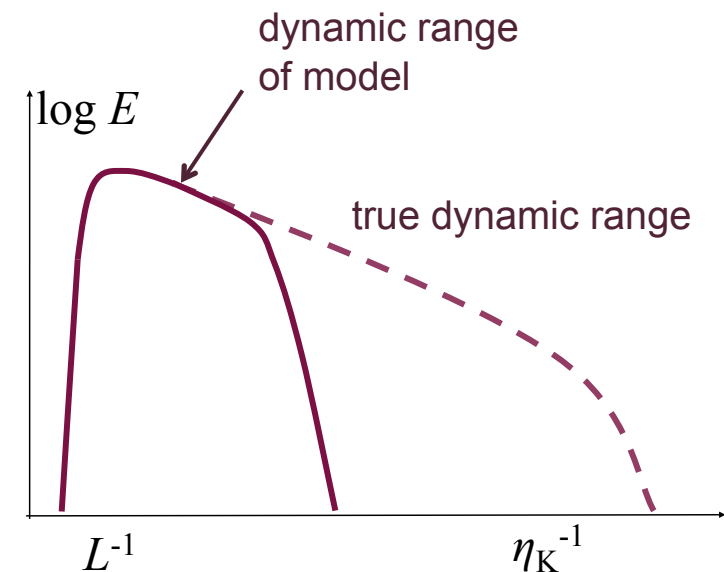
$$\sigma_{\text{rms}} \ll 1 \text{ km/s}$$
$$M_{\text{rms}} \leq 1$$
$$L \approx 0.1 \text{ pc}$$

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



Large-eddy simulations

- We use **LES** to model the large-scale dynamics
- Principal problem: only large scale flow properties
 - Reynolds number: $Re = LV/\nu$ ($Re_{nature} \gg Re_{model}$)
 - dynamic range much smaller than true physical one
 - need **subgrid model** (in our case simple: only dissipation)
 - but what to do for more complex when processes on subgrid scale determine large-scale dynamics (chemical reactions, nuclear burning, etc)
- Turbulence is “space filling” --> difficulty for AMR (don't know what criterion to use for refinement)
- How **large** a Reynolds number do we need to catch basic dynamics right?



See also talks by Norman, Kritsuk, Müller, and others



three examples

- statistics of ISM turbulence
 - rotational vs dilatational modes
- formation of molecular cloud in the turbulent ISM
 - combining MHD with time-dependent chemistry
- the first (strong) B-fields in the universe
 - the turbulent dynamo in action

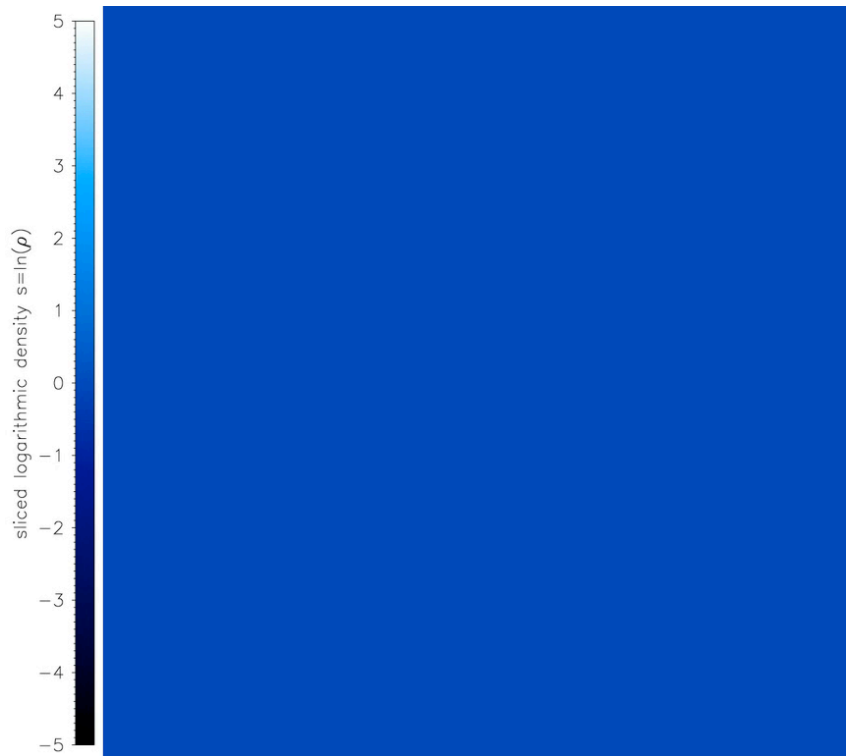


Statistics

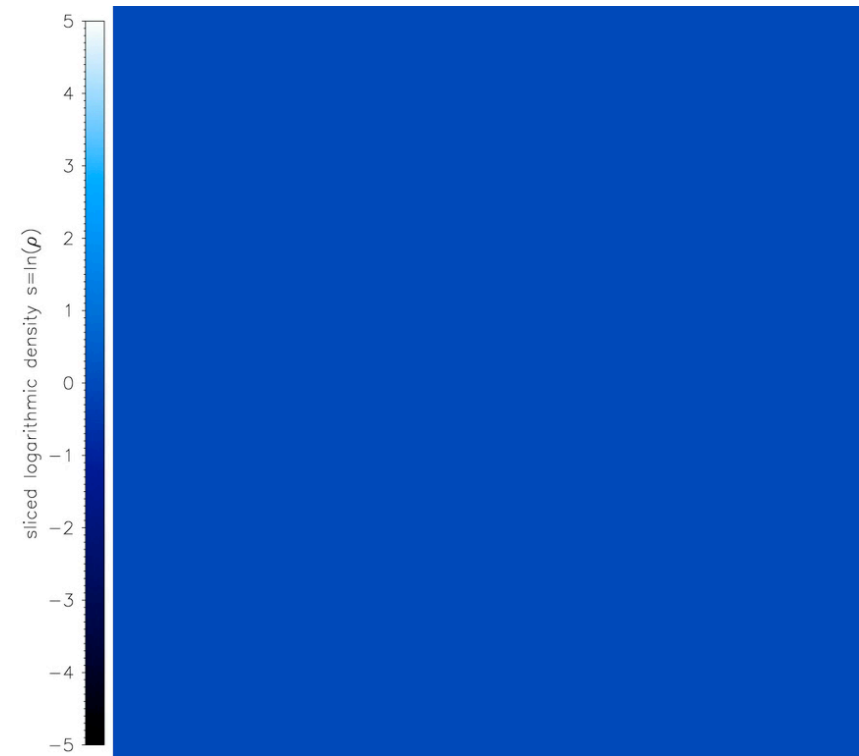


dilatational vs. solenoidal

density as function of time / cut through 1024^3 cube simulation (FLASH)

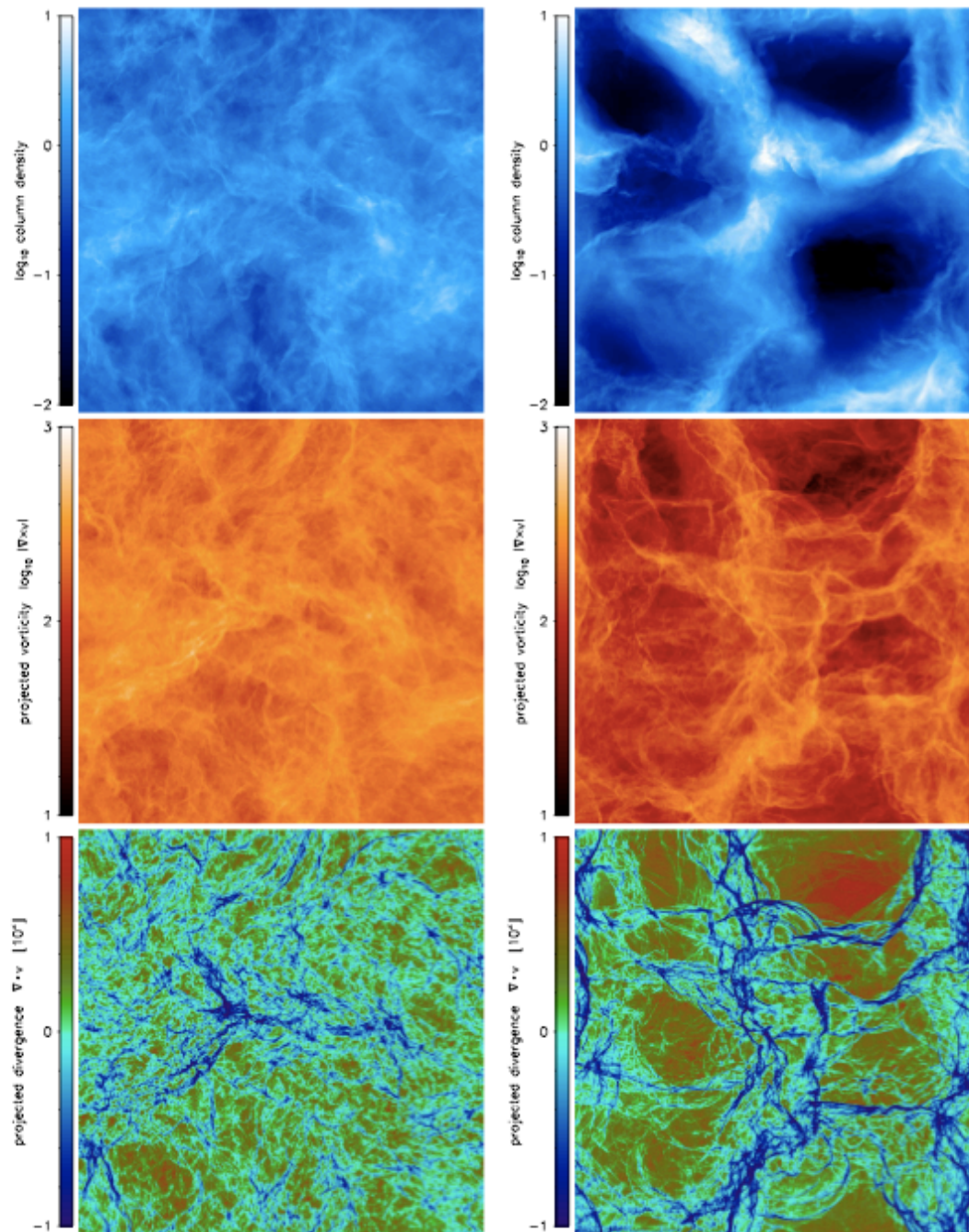


compressive
larger structures, higher ρ -contrast



rotational
smaller structures, small ρ -pdf

Federrath, Klessen, Schmidt (2008a,b)



column density

projected vorticity

projected divergence

Fig. 1. Maps showing density, vorticity and divergence in projection along the z -axis at time $t = 2T$ as an example for the regime of statistically fully developed compressible turbulence for solenoidal forcing (*left*) and compressive forcing (*right*). *Top panels*: Column density fields in units of the mean column density. Both maps show three orders of magnitude in column density with the same scaling and magnitudes for direct comparison. *Middle panels*: Projections of the modulus of the vorticity $|\nabla \times \mathbf{v}|$. Regions of intense vorticity appear to be elongated filamentary structures often coinciding with positions of intersecting shocks. *Bottom panels*: Projections of the divergence of the velocity field $\nabla \cdot \mathbf{v}$ showing the positions of shocks. Negative divergence corresponds to compression, while positive divergence corresponds to rarefaction.



dilatational vs. solenoidal

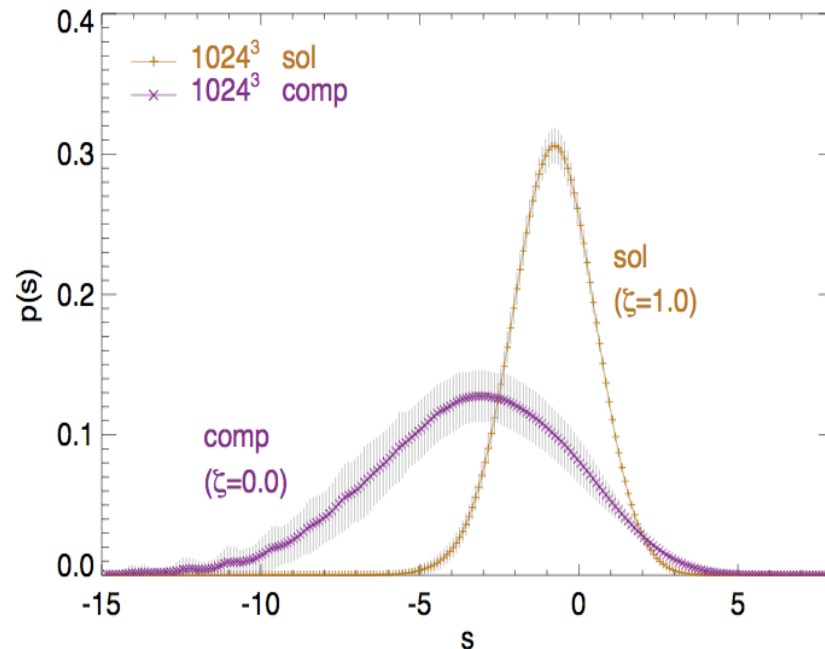


FIG. 2.— Volume-weighted density PDFs $p_s(s)$ in linear scaling where $s = \ln(\rho/\rho_0)$. The PDF obtained by compressive forcing (comp, $\zeta = 0.0$) is much broader compared to the solenoidal one (sol, $\zeta = 1.0$) at the same rms Mach number. The peak is shifted due to mass conservation (Vázquez-Semadeni 1994). Gray error bars indicate 1-sigma temporal fluctuations of the PDF. A sample of $\sim 10^{11}$ datapoints contribute to each PDF.

Federrath, Klessen, Schmidt (2008a)

- density pdf depends on “dimensionality” of driving
- relation between width of pdf and Mach number

$$\sigma_\rho / \rho_0 = b \mathcal{M}$$

- with b depending on ζ via

$$b = 1 + \left[\frac{1}{D} - 1 \right] \zeta = \begin{cases} 1 - \frac{2}{3}\zeta & , \text{ for } D = 3 \\ 1 - \frac{1}{2}\zeta & , \text{ for } D = 2 \\ 1 & , \text{ for } D = 1 \end{cases}$$

- with ζ being the ratio of dilatational vs. solenoidal modes:

$$\mathcal{P}_{ij}^\zeta = \zeta \mathcal{P}_{ij}^\perp + (1 - \zeta) \mathcal{P}_{ij}^\parallel = \zeta \delta_{ij} + (1 - 2\zeta) \frac{k_i k_j}{|k|^2}$$



dilatational vs. solenoidal

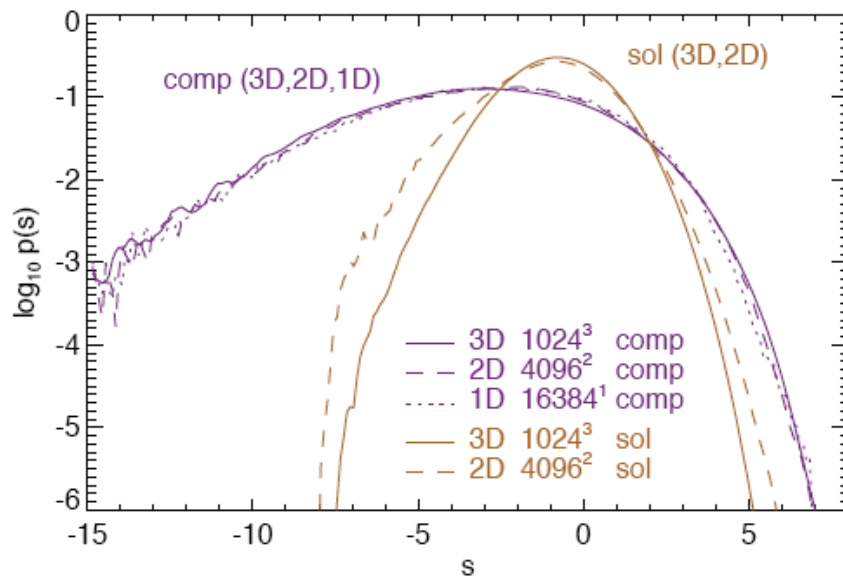


FIG. 3.— Volume-weighted density PDFs $p(s)$ obtained from 3D, 2D and 1D simulations with compressive forcing and from 3D and 2D simulations using solenoidal forcing. Note that in 1D, only compressive forcing is possible as in the study by Passot & Vázquez-Semadeni (1998). As suggested by eq. (5), compressive forcing yields almost identical density PDFs in 1D, 2D and 3D with $b \sim 1$, whereas solenoidal forcing leads to a density PDF with $b \sim 1/2$ in 2D and with $b \sim 1/3$ in 3D.

Federrath, Klessen, Schmidt (2008a)

- density pdf depends on “dimensionality” of driving
- relation between width of pdf and Mach number

$$\sigma_\rho / \rho_0 = b\mathcal{M}$$

- with b depending on ζ via

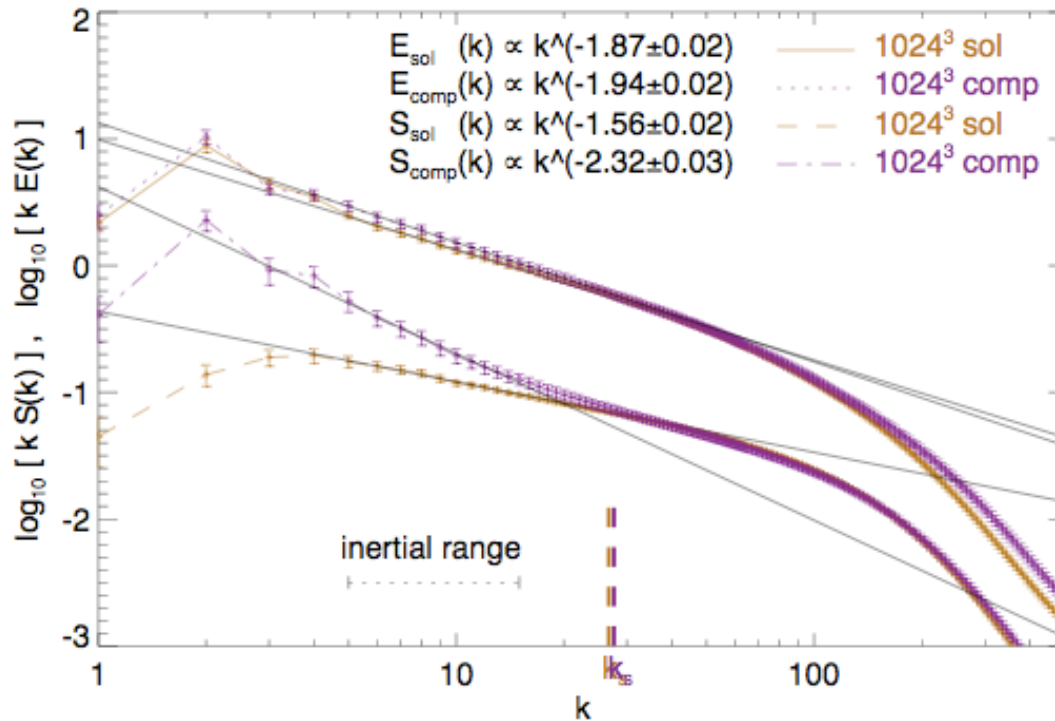
$$b = 1 + \left[\frac{1}{D} - 1 \right] \zeta = \begin{cases} 1 - \frac{2}{3}\zeta & , \text{ for } D = 3 \\ 1 - \frac{1}{2}\zeta & , \text{ for } D = 2 \\ 1 & , \text{ for } D = 1 \end{cases}$$

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dilatational vs. solenoidal



compensated density spectrum $kS(k)$ shows clear break at sonic scale. below that shock compression no longer is important in shaping the power spectrum ...

- density power spectrum differs between dilatational and solenoidal driving!

→ dilatational driving leads to break at sonic scale!

- can we use that to determine driving sources from observations ?



dilatational vs. solenoidal

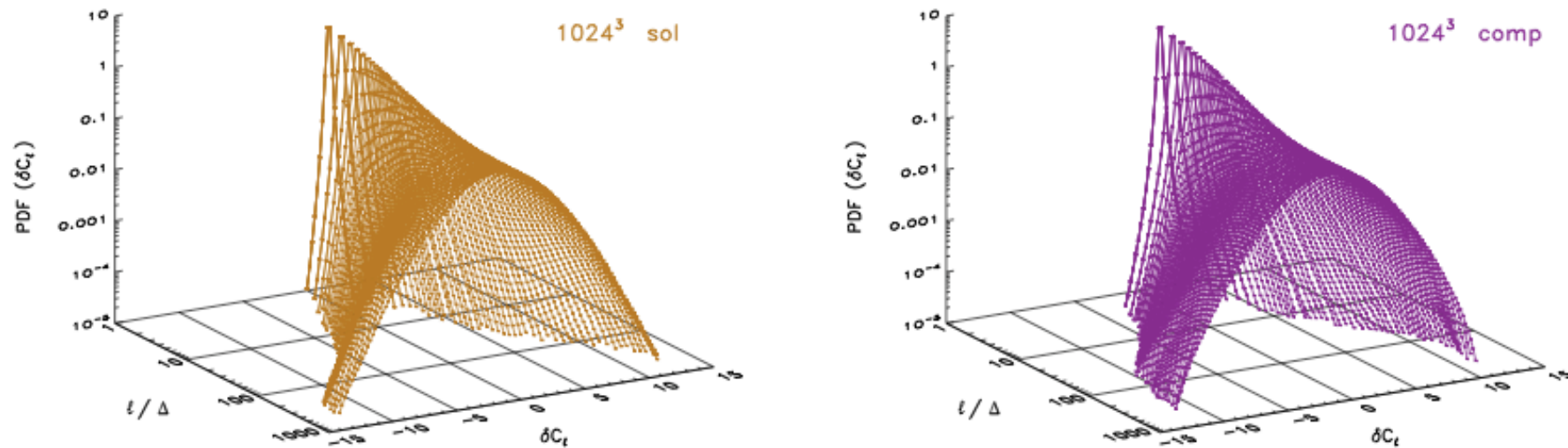


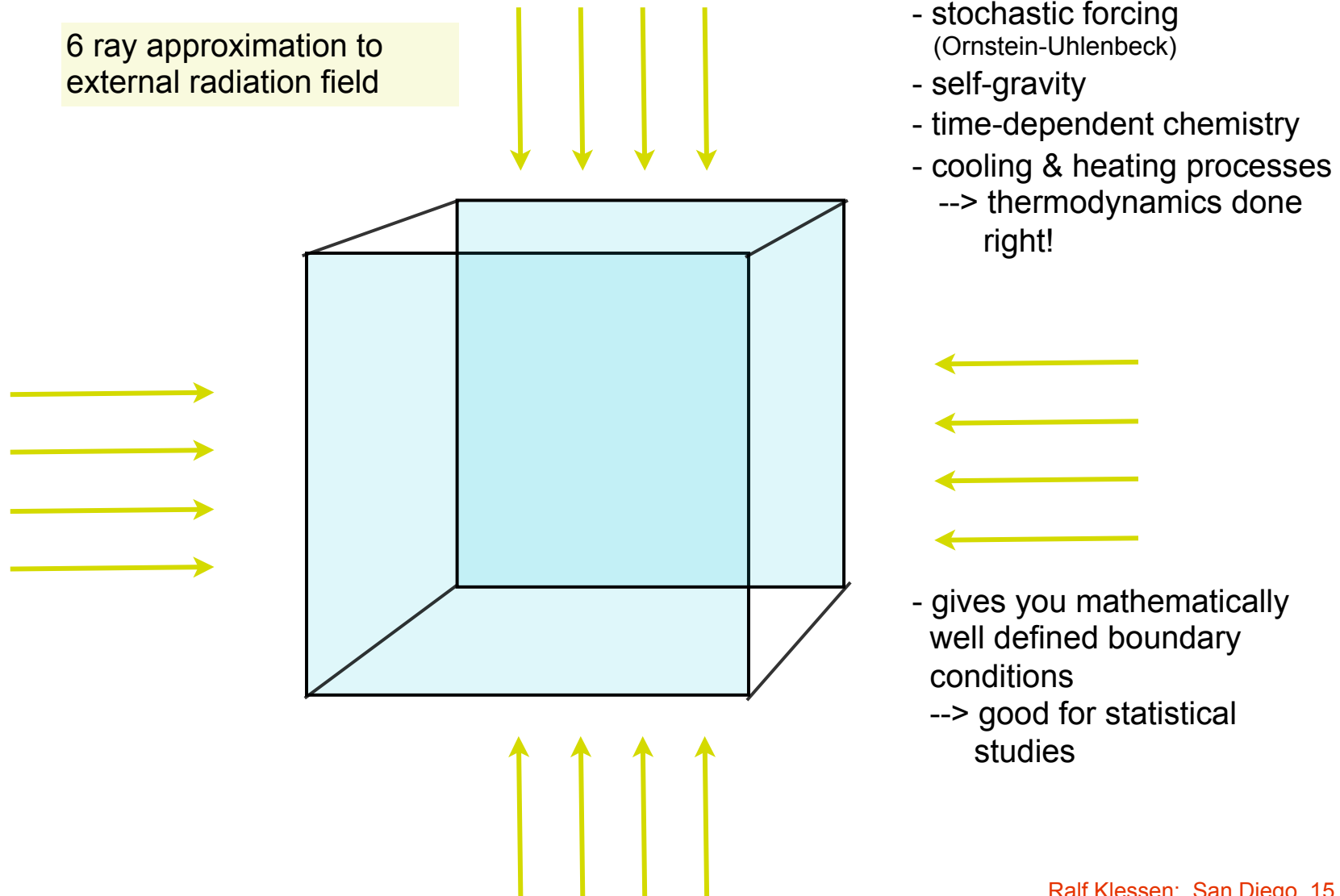
Fig. 7. PDFs of centroid velocity increments computed using equations (18) and (19) are shown as a function of the lag ℓ in units of grid cells $\Delta = L/1024$ for solenoidal forcing (*left*) and compressive forcing (*right*). The PDFs are very close to Gaussian distributions for large lags ℓ , whereas for small lags, they develop exponential tails, which is a manifestation of intermittency (e.g., Hily-Blant et al. 2008).



molecular clouds



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, 17+ heating / cooling processes

- operator-split, implicit method: DVODE

(Brown, Byrne & Hindmarsh 1989)

- extension of consistent multi-fluid advection scheme

(Plewa & Müller 1999)



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) Le Bourlot, Pineau des Forêts & Flower (1999)
H ₂ rovibrational lines	Neufeld & Kaufman (1993); Neufeld, Lepp & Melnick (1995)
CO and H ₂ O rovibrational lines	Pavlovski et al. (2002)
OH rotational lines	Hollenbach & McKee (1989)
Gas-grain energy transfer	Wolfire et al. (2003)
Recombination on grains	Sutherland & Dopita (1993)
Atomic resonance lines	Abel et al. (1997)
H collisional ionization	See Table B1
H ₂ collisional dissociation	Cen (1992)
Compton cooling	

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, MNRAS, 404, 2)



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

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

No.	Reaction			
1	$H + e^- \rightarrow H^- + \gamma$			
2	$H^- + H \rightarrow H_2 + e^-$	$k_2 = 1.5 \times 10^{-9}$ $= 4.0 \times 10^{-9} T^{-0.17}$	$T > 6000$ K $T \leq 300$ K $T > 300$ K	2
3	$H + H^+ \rightarrow H_2^+ + \gamma$	$k_3 = \text{dex}[-19.38 - 1.523 \log T$ $+ 1.118(\log T)^2 - 0.1269(\log T)^3]$		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	$H_2^+ + e^- \rightarrow H + H$	$k_6 = 1.0 \times 10^{-8}$ $= 1.32 \times 10^{-6} T^{-0.76}$	$T \leq 617$ K $T > 617$ K	6
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	$H_2 + H \rightarrow H + H + H$	$k_{9,l} = 6.67 \times 10^{-12} T^{1/2} \exp\left[-\left(1 + \frac{63590}{T}\right)\right]$ $k_{9,h} = 3.52 \times 10^{-9} \exp\left(\frac{-43900}{T}\right)$		9 10
10	$H_2 + H_2 \rightarrow H_2 + H + H$	$n_{cr,H} = \text{dex}\left[3.0 - 0.416 \log\left(\frac{T}{10000}\right) - 0.327 \left\{\log\left(\frac{T}{10000}\right)\right\}^2\right]$ $k_{10,l} = \frac{5.996 \times 10^{-30} T^{4.1881}}{(1.0 + 6.761 \times 10^{-6} T)^{5.8881}} \exp\left(\frac{-54657.4}{T}\right)$ $k_{10,h} = 1.3 \times 10^{-9} \exp\left(\frac{-53300}{T}\right)$ $n_{cr,H_2} = \text{dex}\left[4.845 - 1.3 \log\left(\frac{T}{10000}\right) + 1.62 \left\{\log\left(\frac{T}{10000}\right)\right\}^2\right]$		10 11 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	$H^+ + e^- \rightarrow H + \gamma$	$k_{12,A} = 1.269 \times 10^{-13} \left(\frac{315614}{T}\right)^{1.503}$ $\times [1.0 + \left(\frac{604625}{T}\right)^{0.470}]^{-1.923}$ $k_{12,B} = 2.753 \times 10^{-14} \left(\frac{315614}{T}\right)^{1.500}$ $\times [1.0 + \left(\frac{115188}{T}\right)^{0.457}]^{-2.242}$	Case A Case B	14 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

chemical model 2



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

Table B1.

No. Rea

1 H+

2 H-

3 H+

4 H+

5 H-

6 H₂⁺

7 H₂

8 H₂

9 H₂

10 H₂

11 H+

12 H⁺

13 H-

14	$H^- + H \rightarrow H + H + e^-$	$k_{14} = 2.5634 \times 10^{-9} T_e^{1.78186}$ $= \exp[-2.0372609 \times 10^1$ $+ 1.13944933 \times 10^0 \ln T_e$ $- 1.4210135 \times 10^{-1} (\ln T_e)^2$ $+ 8.4644554 \times 10^{-3} (\ln T_e)^3$ $- 1.327641 \times 10^{-5} (\ln T_e)^4$ $+ 2.172608 \times 10^{-8} (\ln T_e)^5$ $+ 3.530632 \times 10^{-11} (\ln T_e)^6$ $- 2.9850097 \times 10^{-14} (\ln T_e)^7$ $+ 2.4555012 \times 10^{-17} (\ln T_e)^8$ $- 8.0683825 \times 10^{-20} (\ln T_e)^9]$	$T_e \leq 0.1 \text{ eV}$	13
15	$H^- + H^+ \rightarrow H_2^+ + e^-$	$k_{15} = 6.9 \times 10^{-9} T^{-0.35}$ $= 9.6 \times 10^{-7} T^{-0.90}$	$T_e > 0.1 \text{ eV}$ $T \leq 8000 \text{ K}$ $T > 8000 \text{ K}$	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	$He^+ + e^- \rightarrow He + \gamma$	$k_{17,rr,A} = 10^{-11} T^{-0.5} [12.72 - 1.615 \log T$ $- 0.3162 (\log T)^2 + 0.0493 (\log T)^3]$ $k_{17,rr,B} = 10^{-11} T^{-0.5} [11.19 - 1.676 \log T$ $- 0.2852 (\log T)^2 + 0.04433 (\log T)^3]$ $k_{17,di} = 1.9 \times 10^{-3} T^{-1.5} \exp\left(-\frac{473421}{T}\right)$ $\times \left[1.0 + 0.3 \exp\left(-\frac{94684}{T}\right)\right]$	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 18
19	$He + H^+ \rightarrow He^+ + H$	$k_{19} = 1.26 \times 10^{-9} T^{-0.75} \exp\left(-\frac{127500}{T}\right)$ $= 4.0 \times 10^{-37} T^{4.74}$	$T \leq 10000 \text{ K}$ $T > 10000 \text{ K}$	19
20	$C^+ + e^- \rightarrow C + \gamma$	$k_{20} = 4.67 \times 10^{-12} \left(\frac{T}{300}\right)^{-0.6}$ $= 1.23 \times 10^{-17} \left(\frac{T}{300}\right)^{2.49} \exp\left(\frac{21845.6}{T}\right)$ $= 9.62 \times 10^{-8} \left(\frac{T}{300}\right)^{-1.37} \exp\left(\frac{-115786.2}{T}\right)$	$T \leq 7950 \text{ K}$ $7950 \text{ K} < T \leq 21140 \text{ K}$	20
21	$O^+ + e^- \rightarrow O + \gamma$	$k_{21} = 1.30 \times 10^{-10} T^{-0.64}$ $= 1.41 \times 10^{-10} T^{-0.66} + 7.4 \times 10^{-4} T^{-1.5}$ $\times \exp\left(-\frac{175000}{T}\right) [1.0 + 0.062 \times \exp\left(-\frac{145000}{T}\right)]$	$T \leq 400 \text{ K}$ $T > 400 \text{ K}$	21
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	$C + He^+ \rightarrow C^+ + He$	$k_{29} = 8.58 \times 10^{-17} T^{0.757}$ $= 3.25 \times 10^{-17} T^{0.968}$ $= 2.77 \times 10^{-19} T^{1.597}$	$T \leq 200 \text{ K}$ $200 < T \leq 2000 \text{ K}$ $T > 2000 \text{ K}$	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

chemical model 2



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

Table B1.

No. Rea

1 H+

2 H-

3 H+

4 H+

5 H-

6 H₂⁺

7 H₂

8 H₂

9 H₂

10 H₂

11 H+

22 C+

23 O+

24 O+

25 O+

26 O+

27 C+

28 C+

29 C+

13 H-

31 OH

32 HO

33 HO

34 C+

35 CH

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		$CH + O \rightarrow CO + H$	$k_{38} = 6.6 \times 10^{-11}$	$T \leq 2000 \text{ K}$	35
			$= 1.02 \times 10^{-10} \exp\left(-\frac{914}{T}\right)$	$T > 2000 \text{ K}$	36
39		$C_2 + H \rightarrow CH + C$	$k_{39} = 6.0 \times 10^{-11}$		37
40		$C_2 + C \rightarrow C_3 + H$	$k_{40} = 3.5 \times 10^{-10}$		38
41		$CH_2 + O \rightarrow CO + H_2$	$k_{41} = 8.0 \times 10^{-11}$		39
42		$C_2 + O \rightarrow CO + C$	$k_{42} = 5.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.5}$	$T \leq 300 \text{ K}$	40
	15	H-	$= 5.0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.757}$	$T > 300 \text{ K}$	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		$OH + O \rightarrow O_2 + H$	$k_{47} = 3.50 \times 10^{-11}$	$T \leq 261 \text{ K}$	45
			$= 1.77 \times 10^{-11} \exp\left(\frac{178}{T}\right)$	$T > 261 \text{ K}$	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		$O_2 + C \rightarrow CO + O$	$k_{52} = 4.7 \times 10^{-11} \left(\frac{T}{300}\right)^{-0.34}$	$T \leq 295 \text{ K}$	34
			$= 2.48 \times 10^{-12} \left(\frac{T}{300}\right)^{1.54} \exp\left(\frac{613}{T}\right)$	$T > 295 \text{ K}$	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		$H_3^+ + H \rightarrow H_4^+ + H_2$	$k_{55} = 7.7 \times 10^{-9} \exp\left(-\frac{17560}{T}\right)$		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		$CH_2^+ + H_2 \rightarrow CH_3^+ + H$	$k_{63} = 1.0 \times 10^{-9} \exp\left(-\frac{7080}{T}\right)$		28
64		$CH_2^+ + O \rightarrow HCO^+ + H$	$k_{64} = 1.6 \times 10^{-9}$		53
65		$CH_3^+ + H \rightarrow CH_2^+ + H_2$	$k_{65} = 7.0 \times 10^{-10} \exp\left(-\frac{10560}{T}\right)$		28
66		$CH_3^+ + O \rightarrow HCO^+ + H_2$	$k_{66} = 4.0 \times 10^{-10}$		54
67		$C_2 + O^+ \rightarrow CO^+ + C$	$k_{67} = 4.8 \times 10^{-10}$		28
68		$O^+ + H_2 \rightarrow OH^+ + H$	$k_{68} = 1.7 \times 10^{-9}$		55
69		$O + H_2^+ \rightarrow OH^+ + H$	$k_{69} = 1.5 \times 10^{-9}$		28
70		$O + H_3^+ \rightarrow OH^+ + H_2$	$k_{70} = 8.4 \times 10^{-10}$		56
71		$OH + H_3^+ \rightarrow H_2O^+ + H_2$	$k_{71} = 1.3 \times 10^{-9}$		28
72		$OH + C^+ \rightarrow CO^+ + H$	$k_{72} = 7.7 \times 10^{-10}$		28
73		$OH^+ + H_2 \rightarrow H_2O^+ + H$	$k_{73} = 1.01 \times 10^{-9}$		57
74		$H_2O^+ + H_2 \rightarrow H_3O^+ + H$	$k_{74} = 6.4 \times 10^{-10}$		58
75		$H_2O + H_3^+ \rightarrow H_3O^+ + H_2$	$k_{75} = 5.9 \times 10^{-9}$		59
76		$H_2O + C^+ \rightarrow HCO^+ + H$	$k_{76} = 9.0 \times 10^{-10}$		60
77		$H_2O + C^+ \rightarrow HOC^+ + H$	$k_{77} = 1.8 \times 10^{-9}$		60
78		$H_3O^+ + C \rightarrow HCO^+ + H_2$	$k_{78} = 1.0 \times 10^{-11}$		28
79		$O_2 + C^+ \rightarrow CO^+ + O$	$k_{79} = 3.8 \times 10^{-10}$		53
80		$O_2 + C^+ \rightarrow CO + O^+$	$k_{80} = 6.2 \times 10^{-10}$		53
81		$O_2 + CH_2^+ \rightarrow HCO^+ + OH$	$k_{81} = 9.1 \times 10^{-10}$		53
82		$O_3^+ + C \rightarrow CO^+ + O$	$k_{82} = 5.2 \times 10^{-11}$		28
83		$CO + H_3^+ \rightarrow HOC^+ + H_2$	$k_{83} = 2.7 \times 10^{-11}$		61
84		$CO + H_3^+ \rightarrow HCO^+ + H_2$	$k_{84} = 1.7 \times 10^{-9}$		61
85		$HCO^+ + C \rightarrow CO + CH^+$	$k_{85} = 1.1 \times 10^{-9}$		28
86		$HCO^+ + H_2O \rightarrow CO + H_3O^+$	$k_{86} = 2.5 \times 10^{-9}$		62
87					62





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

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-
31	OH
32	HO
33	HO
34	C+
35	CH

14	H ⁻ + H → H + H + e ⁻	88	H ₂ + He ⁺ → He + H ₂ ⁺	k ₈₈ = 7.2 × 10 ⁻¹⁵	63
36	CH + H ₂	89	H ₂ + He ⁺ → He + H + H ⁺	k ₈₉ = 3.7 × 10 ⁻¹⁴ exp($\frac{35}{T}$)	63
37	CH + C	90	CH + H ⁺ → CH ⁺ + H	k ₉₀ = 1.9 × 10 ⁻⁹	28
38	CH + O	91	CH ₂ + H ⁺ → CH ₂ ⁺ + H	k ₉₁ = 1.4 × 10 ⁻⁹	28
39	C ₂ + H	92	CH ₂ + H ⁺ → C ⁺ + He + H ₂	k ₉₂ = 7.5 × 10 ⁻¹⁰	28
40	C ₂ + C	93	OH + H ⁺ → OH ⁺ + H	k ₉₃ = 1.1 × 10 ⁻⁹	28
41	CH ₂ + O	94	OH + H ⁺ → OH ⁺ + H	k ₉₄ = 1.1 × 10 ⁻⁹	28
42	C ₂ + O →	95	OH + H ⁺ → OH ⁺ + H	k ₉₅ = 1.1 × 10 ⁻⁹	28
15	H ⁻	96	H ₂ O + H ⁺ → H ₂ O ⁺ + H	k ₉₆ = 6.9 × 10 ⁻⁹	64
16	He	97	H ₂ O + He ⁺ → OH + He + H ⁺	k ₉₇ = 2.04 × 10 ⁻¹⁰	65
43	O + H ₂ →	98	H ₂ O + He ⁺ → OH ⁺ + He + H	k ₉₈ = 2.86 × 10 ⁻¹⁰	65
44	OH + H	99	H ₂ O + He ⁺ → H ₂ O ⁺ + He	k ₉₉ = 6.05 × 10 ⁻¹¹	65
45	OH + H ₂	100	O ₂ + H ⁺ → O ₂ ⁺ + H	k ₁₀₀ = 2.0 × 10 ⁻⁹	64
46	OH + C	101	O ₂ + He ⁺ → O ₂ ⁺ + He	k ₁₀₁ = 3.3 × 10 ⁻¹¹	66
47	OH + O	102	O ₂ + He ⁺ → O ⁺ + O + He	k ₁₀₂ = 1.1 × 10 ⁻⁹	66
48	OH + OH	103	O ₂ ⁺ + C → O ₂ + C ⁺	k ₁₀₃ = 5.2 × 10 ⁻¹¹	28
49	H ₂ O + H	104	CO + He ⁺ → C ⁺ + O + He	k ₁₀₄ = 1.4 × 10 ⁻⁹ ($\frac{T}{300}$) ^{-0.5}	67
50	O ₂ + H →	105	CO + He ⁺ → C + O ⁺ + He	k ₁₀₅ = 1.4 × 10 ⁻¹⁶ ($\frac{T}{300}$) ^{-0.5}	67
51	O ₂ + H ₂	106	CO ⁺ + H → CO + H ⁺	k ₁₀₆ = 7.5 × 10 ⁻¹⁰	68
52	O ₂ + C →	107	C ⁻ + H ⁺ → C + H	k ₁₀₇ = 2.3 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.5}	28
53	CO + H	108	O ⁻ + H ⁺ → O + H	k ₁₀₈ = 2.3 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.5}	28
54	H ₃ ⁺ + H ₂	109	He ⁺ + H ⁻ → He + H	k ₁₀₉ = 2.32 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.52} exp($\frac{T}{22400}$)	69
55	H ₃ ⁺ + H	110	H ₃ ⁺ + e ⁻ → H ₂ + H	k ₁₁₀ = 2.34 × 10 ⁻⁸ ($\frac{T}{300}$) ^{-0.52}	70
56	C + H ₂ ⁺	111	H ₃ ⁺ + e ⁻ → H + H + H	k ₁₁₁ = 4.36 × 10 ⁻⁸ ($\frac{T}{300}$) ^{-0.52}	70
57	C + H ₃ ⁺	112	CH ⁺ + e ⁻ → C + H	k ₁₁₂ = 7.0 × 10 ⁻⁸ ($\frac{T}{300}$) ^{-0.5}	71
58	C ⁺ + H ₂	113	CH ₂ ⁺ + e ⁻ → CH + H	k ₁₁₃ = 1.6 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.6}	72
59	CH ⁺ + H	114	CH ₂ ⁺ + e ⁻ → C + H + H	k ₁₁₄ = 4.03 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.6}	72
60	CH ⁺ + H ₂	115	CH ₂ ⁺ + e ⁻ → C + H ₂	k ₁₁₅ = 7.68 × 10 ⁻⁸ ($\frac{T}{300}$) ^{-0.6}	72
61	CH ⁺ + O	116	CH ₃ ⁺ + e ⁻ → CH ₂ + H	k ₁₁₆ = 7.75 × 10 ⁻⁸ ($\frac{T}{300}$) ^{-0.5}	73
62	CH ₂ ⁺ + H ⁺	117	CH ₃ ⁺ + e ⁻ → CH + H ₂	k ₁₁₇ = 1.95 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.5}	73
63	CH ₂ ⁺ + H	118	CH ₃ ⁺ + e ⁻ → CH + H + H	k ₁₁₈ = 2.0 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.4}	28
64	CH ₂ ⁺ + H ₂	119	OH ⁺ + e ⁻ → O + H	k ₁₁₉ = 6.3 × 10 ⁻⁹ ($\frac{T}{300}$) ^{-0.48}	74
65	CH ₂ ⁺ + O	120	H ₂ O ⁺ + e ⁻ → O + H + H	k ₁₂₀ = 3.05 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.5}	75
66	CH ₃ ⁺ + H	121	H ₂ O ⁺ + e ⁻ → O + H ₂	k ₁₂₁ = 3.9 × 10 ⁻⁸ ($\frac{T}{300}$) ^{-0.5}	75
67	CH ₃ ⁺ + O	122	H ₂ O ⁺ + e ⁻ → OH + H	k ₁₂₂ = 8.6 × 10 ⁻⁸ ($\frac{T}{300}$) ^{-0.5}	75
68	C ₂ + O ⁺	123	H ₃ O ⁺ + e ⁻ → H + H ₂ O	k ₁₂₃ = 1.08 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.5}	76
69	O ⁺ + H ₂	124	H ₃ O ⁺ + e ⁻ → OH + H ₂	k ₁₂₄ = 6.02 × 10 ⁻⁸ ($\frac{T}{300}$) ^{-0.5}	76
70	O + H ₂ ⁺	125	H ₃ O ⁺ + e ⁻ → OH + H + H	k ₁₂₅ = 2.58 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.5}	76
71	O + H ₃ ⁺	126	H ₃ O ⁺ + e ⁻ → O + H + H ₂	k ₁₂₆ = 5.6 × 10 ⁻⁹ ($\frac{T}{300}$) ^{-0.5}	76
72	OH + H ₃ ⁺	127	O ₂ ⁺ + e ⁻ → O + O	k ₁₂₇ = 1.95 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.7}	77
73	OH + C ⁺	128	CO ⁺ + e ⁻ → C + O	k ₁₂₈ = 2.75 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.55}	78
74	OH ⁺ + H ₂	129	HCO ⁺ + e ⁻ → CO + H	k ₁₂₉ = 2.76 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-0.64}	79
75	H ₂ O ⁺ + H	130	HCO ⁺ + e ⁻ → OH + C	k ₁₃₀ = 2.4 × 10 ⁻⁸ ($\frac{T}{300}$) ^{-0.64}	79
76	H ₂ O ⁺ + C	131	HOC ⁺ + e ⁻ → CO + H	k ₁₃₁ = 1.1 × 10 ⁻⁷ ($\frac{T}{300}$) ^{-1.0}	28
77	H ₂ O + C ⁺	132	H ⁻ + C → CH + e ⁻	k ₁₃₂ = 1.0 × 10 ⁻⁹	28
78	H ₃ O ⁺ + C	133	H ⁻ + O → OH + e ⁻	k ₁₃₃ = 1.0 × 10 ⁻⁹	28
79	O ₂ + C ⁺	134	H ⁻ + OH → H ₂ O + e ⁻	k ₁₃₄ = 1.0 × 10 ⁻¹⁰	28
80	O ₂ + C ⁺	135	C ⁻ + H → CH + e ⁻	k ₁₃₅ = 5.0 × 10 ⁻¹⁰	28
81	O ₂ + C ⁺	136	C ⁻ + H ₂ → CH ₂ + e ⁻	k ₁₃₆ = 1.0 × 10 ⁻¹³	28
82	O ₂ + CH ₂ ⁺	137	C ⁻ + O → CO + e ⁻	k ₁₃₇ = 5.0 × 10 ⁻¹⁰	28
83	O ₂ ⁺ + C	138	O ⁻ + H → OH + e ⁻	k ₁₃₈ = 5.0 × 10 ⁻¹⁰	28
84	CO + H ₃ ⁺	139	O ⁻ + H ₂ → H ₂ O + e ⁻	k ₁₃₉ = 7.0 × 10 ⁻¹⁰	28
85	CO + H ₃ ⁺	140	O ⁻ + C → CO + e ⁻	k ₁₄₀ = 5.0 × 10 ⁻¹⁰	28
86	HCO ⁺ + C				
87	HCO ⁺ + H ₃ O ⁺ → CO + H ₃ O ⁺	k ₈₇ = 2.5 × 10 ⁻¹⁰			62

chemical model 2



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

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 → H + H + e ⁻	88	H ₂ + He ⁺ → He + H ₂ ⁺	k ₈₈ = 7.2 × 10 ⁻¹⁵	63
36	CH + H ₂	89	H ₂ + He ⁺ → He + H + H ⁺	k ₈₉ = 3.7 × 10 ⁻¹⁴ exp(35/T)	63
37	CH + C	90	CH + H ⁺ → CH ⁺ + H	k ₉₀ = 1.9 × 10 ⁻⁹	28
38	CH + O	91	CH ₂ + H ⁺ → CH ₂ ⁺ + H	k ₉₁ = 1.4 × 10 ⁻⁹	28
39	C ₂ + H ⁺	92	CH ₂ + H ⁺ → C ⁺ + He + H ₂	k ₉₂ = 7.5 × 10 ⁻¹⁰	28
40	C ₂ + C	93	OH + H ⁺ → OH ⁺ + H	k ₉₃ = 1.1 × 10 ⁻⁹	28
41	CH ₂ + O	94	OH + H ₂ → H ₂ O + H	k ₉₄ = 1.1 × 10 ⁻⁹	28
42	C ₂ + O →	95	H ₂ O + H ⁺ → H ₂ O ⁺ + H	k ₉₅ = 1.1 × 10 ⁻⁹	28
43	O + H ₂ →	96	H ₂ O + H ⁺ → H ₂ O ⁺ + H	k ₉₆ = 6.9 × 10 ⁻⁹	64
44	OH + H	97	H ₂ O + He ⁺ → OH + He + H ⁺	k ₉₇ = 2.04 × 10 ⁻¹⁰	65
45	OH + H ₂	98	H ₂ O + H ₂ ⁺ → OH ⁺ + H ₂ + H	k ₉₈ = 2.04 × 10 ⁻¹⁰	65
46	OH + C	99	C + e ⁻ → C ⁻ + γ	k ₁₄₂ = 2.25 × 10 ⁻¹⁵	81
47	OH + O	100	C + H → CH + γ	k ₁₄₃ = 1.0 × 10 ⁻¹⁷	82
48	OH + OH	101	C + H ₂ → CH ₂ + γ	k ₁₄₄ = 1.0 × 10 ⁻¹⁷	82
49	H ₂ O + H	102	C + C → C ₂ + γ	k ₁₄₅ = 4.36 × 10 ⁻¹⁸ (T/300) ^{0.35} exp(-161.3/T)	83
50	O ₂ + H	103	C + O → CO + γ	k ₁₄₆ = 2.1 × 10 ⁻¹⁹	T ≤ 300 K 84
51	O ₂ + H ₂	104	C ⁺ + H → CH ⁺ + γ	= 3.09 × 10 ⁻¹⁷ (T/300) ^{0.33} exp(-1629/T)	T > 300 K 85
52	O ₂ + C →	105	C ⁺ + H ₂ → CH ₂ ⁺ + γ	k ₁₄₇ = 4.46 × 10 ⁻¹⁶ T ^{-0.5} exp(-4.93/T ^{2/3})	86
53	CO + H	106	C ⁺ + O → CO ⁺ + γ	k ₁₄₈ = 4.0 × 10 ⁻¹⁶ (T/300) ^{-0.2}	87
54	H ₂ ⁺ + H ₂	107	O + e ⁻ → O ⁻ + γ	k ₁₄₉ = 2.5 × 10 ⁻¹⁸	T ≤ 300 K 84
55	H ₃ ⁺ + H	108	O + H → OH + γ	= 3.14 × 10 ⁻¹⁸ (T/300) ^{-0.15} exp(68/T)	T > 300 K 84
56	C + H ₂ ⁺	109	O + O → O ₂ + γ	k ₁₅₀ = 1.5 × 10 ⁻¹⁵	28
57	C + H ₃ ⁺	110	OH + H → H ₂ O + γ	k ₁₅₁ = 9.9 × 10 ⁻¹⁹ (T/300) ^{-0.38}	28
58	C ⁺ + H ₂	111	H + H + H → H ₂ + H	k ₁₅₂ = 4.9 × 10 ⁻²⁰ (T/300) ^{1.58}	82
59	CH ⁺ + H	112	H + H + H ₂ → H ₂ + H ₂	k ₁₅₃ = 5.26 × 10 ⁻¹⁸ (T/300) ^{-5.22} exp(-90/T)	88
60	CH ⁺ + H ₂	113	H + H + He → H ₂ + He	k ₁₅₄ = 1.32 × 10 ⁻³² (T/300) ^{-0.38}	T ≤ 300 K 89
61	CH ⁺ + O	114	C + C + M → C ₂ + M	= 1.32 × 10 ⁻³² (T/300) ^{-1.0}	T > 300 K 90
62	CH ₂ ⁺ + H ⁺	115	C + O + M → CO + M	k ₁₅₅ = 2.8 × 10 ⁻³¹ T ^{-0.6}	91
63	CH ₂ ⁺ + H	116	C + O + M → CO + M	k ₁₅₆ = 6.9 × 10 ⁻³² T ^{-0.4}	92
64	CH ₂ ⁺ + H ₂	117	C ⁺ + O + M → CO ⁺ + M	k ₁₅₇ = 5.99 × 10 ⁻³³ (T/5000) ^{-1.6}	T ≤ 5000 K 93
65	CH ₂ ⁺ + O	118	C + O + M → CO + M	= 5.99 × 10 ⁻³³ (T/5000) ^{-0.64} exp(5255/T)	T > 5000 K 94
66	CH ₃ ⁺ + H	119	C ⁺ + O + M → CO ⁺ + M	k ₁₅₈ = 6.16 × 10 ⁻²⁹ (T/300) ^{-3.08}	T ≤ 2000 K 35
67	CH ₃ ⁺ + O	120	C + O + M → CO + M	= 2.14 × 10 ⁻²⁹ (T/300) ^{-3.08} exp(2114/T)	T > 2000 K 67
68	C ₂ + O ⁺	121	C ⁺ + O + M → CO ⁺ + M	k ₁₅₉ = 100 × k ₂₁₀	67
69	O ⁺ + H ₂	122	C + O ⁺ + M → CO ⁺ + M	k ₁₆₀ = 100 × k ₂₁₀	67
70	O + H ₂ ⁺	123	O + H + M → OH + M	k ₁₆₁ = 4.33 × 10 ⁻³² (T/300) ^{-1.0}	43
71	O + H ₃ ⁺	124	OH + H + M → H ₂ O + M	k ₁₆₂ = 2.56 × 10 ⁻³¹ (T/300) ^{-2.0}	35
72	OH + H ₃ ⁺	125	O + O + M → O ₂ + M	k ₁₆₃ = 9.2 × 10 ⁻³⁴ (T/300) ^{-1.0}	37
73	OH + C ⁺	126	O + O + M → O ₂ + M	k ₁₆₄ = 2.0 × 10 ⁻¹¹ (T/300) ^{0.44}	95
74	OH ⁺ + H ₂	127	O + CH → HCO ⁺ + e ⁻	k ₁₆₅ = 3.0 × 10 ⁻¹⁸ T ^{0.5} f _A [1.0 + 0.04(T + T _d) ^{0.5} + 0.002 T + 8 × 10 ⁻⁶ T ²] ⁻¹	f _A = [1.0 + 10 ⁴ exp(-600/T _d)] ⁻¹ 96
75	H ₂ O ⁺ + H	128	H + H(s) → H ₂		
76	H ₂ O + H ₃ ⁺	129	HCO ⁺ + e ⁻ → CO + H	k ₁₂₉ = 2.76 × 10 ⁻⁷ (T/300) ^{-0.64}	79
77	H ₂ O + C ⁺	130	HCO ⁺ + e ⁻ → OH + C	k ₁₃₀ = 2.4 × 10 ⁻⁸ (T/300) ^{-0.64}	79
78	H ₂ O + C ⁺	131	HOC ⁺ + e ⁻ → CO + H	k ₁₃₁ = 1.1 × 10 ⁻⁷ (T/300) ^{-1.0}	28
79	H ₃ O ⁺ + C	132	H ⁻ + C → CH + e ⁻	k ₁₃₂ = 1.0 × 10 ⁻⁹	28
80	O ₂ + C ⁺	133	H ⁻ + O → OH + e ⁻	k ₁₃₃ = 1.0 × 10 ⁻⁹	28
81	O ₂ + C ⁺	134	H ⁻ + OH → H ₂ O + e ⁻	k ₁₃₄ = 1.0 × 10 ⁻¹⁰	28
82	O ₂ + CH ₂	135	C ⁻ + H → CH + e ⁻	k ₁₃₅ = 5.0 × 10 ⁻¹⁰	28
83	O ₂ ⁺ + C	136	C ⁻ + H ₂ → CH ₂ + e ⁻	k ₁₃₆ = 1.0 × 10 ⁻¹³	28
84	CO + H ₃ ⁺	137	C ⁻ + O → CO + e ⁻	k ₁₃₇ = 5.0 × 10 ⁻¹⁰	28
85	CO + H ₃ ⁺	138	O ⁻ + H → OH + e ⁻	k ₁₃₈ = 5.0 × 10 ⁻¹⁰	28
86	HCO ⁺ + C	139	O ⁻ + H ₂ → H ₂ O + e ⁻	k ₁₃₉ = 7.0 × 10 ⁻¹⁰	28
87	HCO ⁺ + H ₃ O ⁺ → CO + H ₃ O ⁺	140	O ⁻ + C → CO + e ⁻	k ₁₄₀ = 5.0 × 10 ⁻¹⁰	28

chemical model 2



Table B1.

No.	Rea
1	H +

14	$H^- + H \rightarrow H + H + e^-$	88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$	63
36	$CH + H_2$	89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$	63
37	$CH + C$	90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$	28
38	$CH + O$	91	$CH_2 + H^+ \rightarrow CH_2^+ + H$	$k_{91} = 1.4 \times 10^{-9}$	28
		92	$CH_2 + H^+ \rightarrow C^+ + He + H_2$	$k_{92} = 7.5 \times 10^{-10}$	28
39	$C_2 + e^-$				28
40	$C_2 + C$				28
41	$CH_2 + O$				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	$H_2O + H_2^+ \rightarrow OH^+ + H_2 + H$		65

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

25×10^{-15}	81
0×10^{-17}	82
0×10^{-17}	82
$36 \times 10^{-18} \left(\frac{T}{300}\right)^{0.35} \exp\left(-\frac{161.3}{T}\right)$	83
1×10^{-19}	$T \leq 300$ K
$09 \times 10^{-17} \left(\frac{T}{300}\right)^{0.33} \exp\left(-\frac{1629}{T}\right)$	$T > 300$ K
$46 \times 10^{-16} T^{-0.5} \exp\left(-\frac{4.93}{T^{2/3}}\right)$	86
$0 \times 10^{-16} \left(\frac{T}{300}\right)^{-0.2}$	87
5×10^{-18}	$T \leq 300$ K
$14 \times 10^{-18} \left(\frac{T}{300}\right)^{-0.15} \exp\left(\frac{68}{T}\right)$	$T > 300$ K
5×10^{-15}	28
$9 \times 10^{-19} \left(\frac{T}{300}\right)^{-0.38}$	28
$9 \times 10^{-20} \left(\frac{T}{300}\right)^{1.58}$	82
$26 \times 10^{-18} \left(\frac{T}{300}\right)^{-5.22} \exp\left(-\frac{90}{T}\right)$	88
$32 \times 10^{-32} \left(\frac{T}{300}\right)^{-0.38}$	$T \leq 300$ K
$32 \times 10^{-32} \left(\frac{T}{300}\right)^{-1.0}$	$T > 300$ K
$8 \times 10^{-31} T^{-0.6}$	91
$9 \times 10^{-32} T^{-0.4}$	92
$99 \times 10^{-33} \left(\frac{T}{5000}\right)^{-1.6}$	$T \leq 5000$ K
$99 \times 10^{-33} \left(\frac{T}{5000}\right)^{-0.64} \exp\left(\frac{5255}{T}\right)$	$T > 5000$ K
$16 \times 10^{-29} \left(\frac{T}{300}\right)^{-3.08}$	$T \leq 2000$ K
$14 \times 10^{-29} \left(\frac{T}{300}\right)^{-3.08} \exp\left(\frac{2114}{T}\right)$	$T > 2000$ K
$10 \times k_{210}$	67
$10 \times k_{210}$	67
$33 \times 10^{-32} \left(\frac{T}{300}\right)^{-1.0}$	43
$56 \times 10^{-31} \left(\frac{T}{300}\right)^{-2.0}$	35
$2 \times 10^{-34} \left(\frac{T}{300}\right)^{-1.0}$	37
$0 \times 10^{-11} \left(\frac{T}{300}\right)^{0.44}$	95
$0 \times 10^{-18} T^{0.5} f_{\Lambda} [1.0 + 0.04(T + T_d)]^{0.5} f_{\Lambda} = [1.0 + 10^4 \exp(-\frac{600}{T_d})]^{-1}$	96
$0.002 T + 8 \times 10^{-6} T^2]^{-1}$	
$6 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.64}$	79
$\times 10^{-8} \left(\frac{T}{300}\right)^{-0.64}$	79
$\times 10^{-7} \left(\frac{T}{300}\right)^{-1.0}$	28
$\times 10^{-9}$	28
$\times 10^{-9}$	28
$\times 10^{-10}$	28
$\times 10^{-10}$	28
$\times 10^{-13}$	28
$\times 10^{-10}$	28
$\times 10^{-10}$	28
$\times 10^{-10}$	28
$\times 10^{-10}$	28
$\times 10^{-10}$	28

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

86	$HCO^+ + C$	140	$O^- + C \rightarrow CO + e^-$	$k_{140} = 5.0 \times 10^{-10}$	28
87	$HCO^+ + H_3O^+$		$\rightarrow CO + H_3O^+$	$k_{87} = 2.5 \times 10^{-10}$	28



Table B1.

No.	Reaction
1	H + ...

14	$H^- + H \rightarrow H + H + e^-$	88	$H_2 + He^+ \rightarrow He + H_2^+$	$k_{88} = 7.2 \times 10^{-15}$	63
36	$CH + H_2$	89	$H_2 + He^+ \rightarrow He + H + H^+$	$k_{89} = 3.7 \times 10^{-14} \exp\left(\frac{35}{T}\right)$	63
37	$CH + C$	90	$CH + H^+ \rightarrow CH^+ + H$	$k_{90} = 1.9 \times 10^{-9}$	28
38	$CH + O$	91	$CH_2 + H^+ \rightarrow CH_2^+ + H$	$k_{91} = 1.4 \times 10^{-9}$	28
39	$CH_2 + H$	92	$CH_2 + H^+ \rightarrow C^+ + He + H_2$	$k_{92} = 7.5 \times 10^{-10}$	28
40	$CH_2 + C$	94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 1.1 \times 10^{-9}$	28
41	$CH_2 + O$	95	$OH + H^+ \rightarrow OH^+ + H$	$k_{95} = 1.2 \times 10^{-9}$	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	$H_2O + He^+ \rightarrow OH^+ + He + H$	$k_{98} = 2.66 \times 10^{-10}$	65

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	$C + \gamma \rightarrow C^+ + e^-$	$R_{171} = 2.1 \times 10^{-10}$	2.2	2	25×10^{-15}	81
172	$C^- + \gamma \rightarrow$				0×10^{-17}	82
173	$CH + \gamma \rightarrow$				0×10^{-17}	82
174	$CH + \gamma \rightarrow$				$36 \times 10^{-18} \left(\frac{T}{300}\right)^{0.35} \exp\left(-\frac{161.3}{T}\right)$	83
175	$CH^+ + \gamma \rightarrow$				1×10^{-19}	84
176	$CH_2 + \gamma \rightarrow$				$09 \times 10^{-17} \left(\frac{T}{300}\right)^{0.33} \exp\left(-\frac{1629}{T}\right)$	85
177	$CH_2 + \gamma \rightarrow$				$46 \times 10^{-16} T^{-0.5} \exp\left(-\frac{4.93}{T^{2/3}}\right)$	86
178	$CH_2^+ + \gamma \rightarrow$				$0 \times 10^{-16} \left(\frac{T}{300}\right)^{-0.2}$	87
179	$CH_3^+ + \gamma \rightarrow$				5×10^{-18}	84
180	$CH_3^+ + \gamma \rightarrow$				$14 \times 10^{-18} \left(\frac{T}{300}\right)^{-0.15} \exp\left(\frac{68}{T}\right)$	84

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

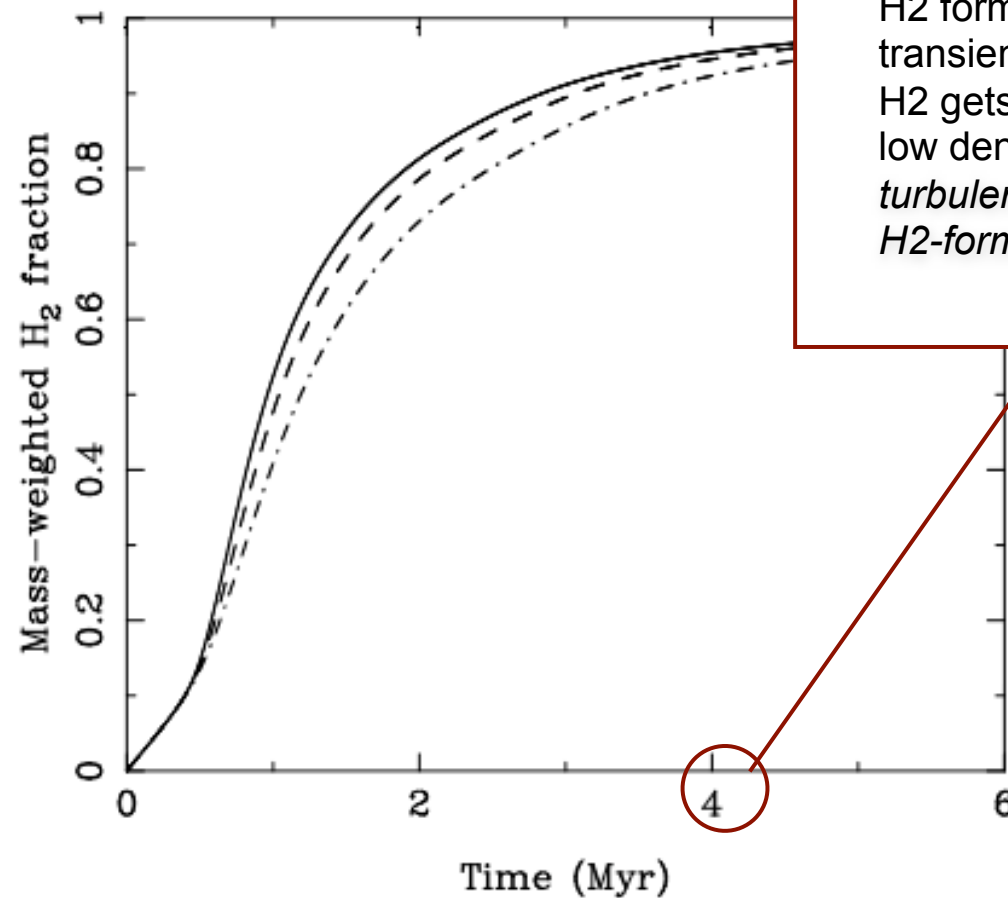
No.	Reaction	Rate ($s^{-1} \zeta_H^{-1}$)	Ref.
199	$H + c.r. \rightarrow H^+ + e^-$	$R_{199} = 1.0$	—
200	$He + c.r. \rightarrow He^+ + e^-$	$R_{200} = 1.1$	1
201	$H_2 + c.r. \rightarrow H^+ + H + e^-$	$R_{201} = 0.037$	1
202	$H_2 + c.r. \rightarrow H + H$	$R_{202} = 0.22$	1
203	$H_2 + c.r. \rightarrow H^+ + H^-$	$R_{203} = 6.5 \times 10^{-4}$	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
197	$O_2 + \gamma \rightarrow O + O$	$R_{197} = 7.0 \times 10^{-10}$	7
198	$CO + \gamma \rightarrow C + O$	$R_{198} = 2.0 \times 10^{-10}$	13

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

86	$HCO^+ + C$	140	$O^- + C \rightarrow CO + e^-$	$k_{140} = 5.0 \times 10^{-10}$	28
87	$HCO^+ + H_3O \rightarrow CO + H_3O^+$	$k_{87} = 2.5 \times 10^{-10}$			28



HI to H₂ conversion rate



H₂ forms rapidly in shocks / transient density fluctuations / H₂ gets destroyed slowly in low density regions / result: *turbulence greatly enhances H₂-formation rate*

Figure 4. Time evolution of the mass-weighted H₂ abundance in simulations R1, R2 and R3, which have numerical resolutions of 64³ zones (dot-dashed), 128³ zones (dashed) and 256³ zones (solid), respectively.



CO, C⁺ formation rates

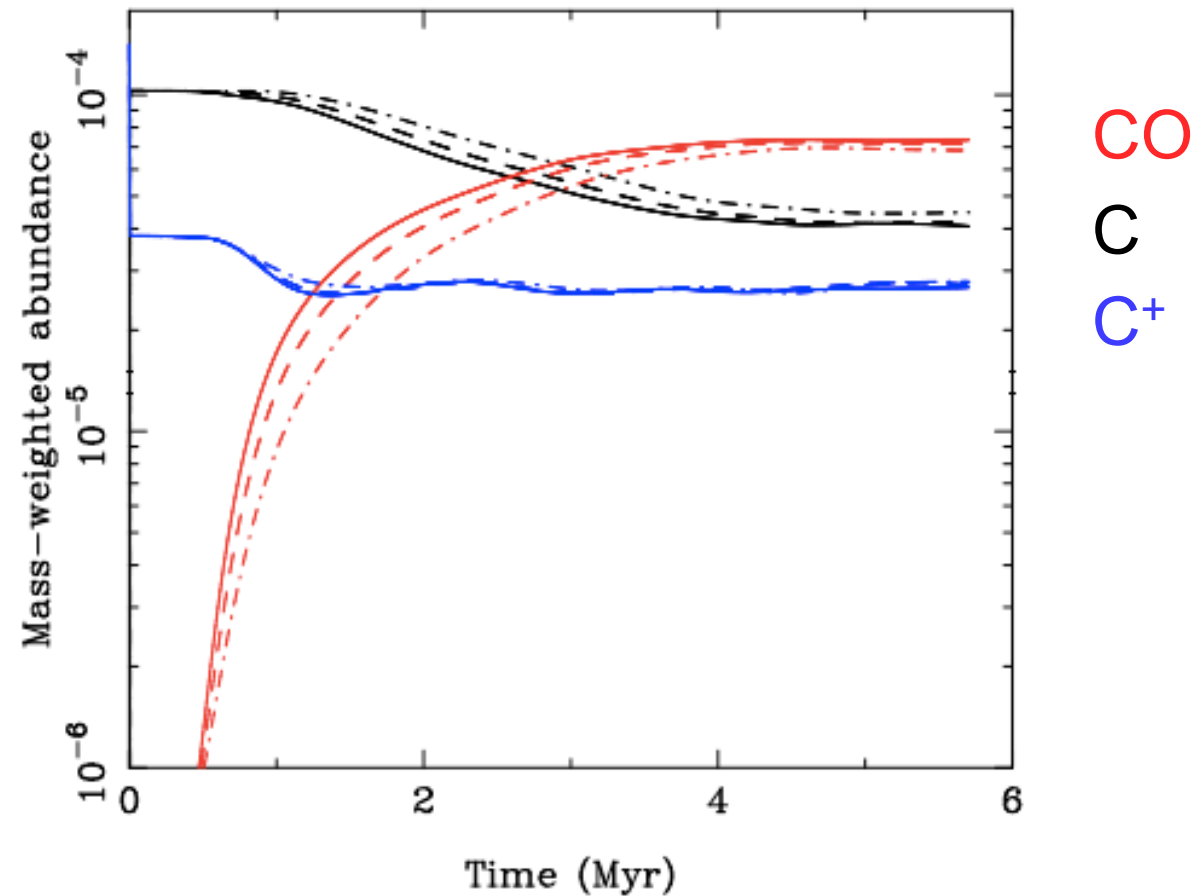
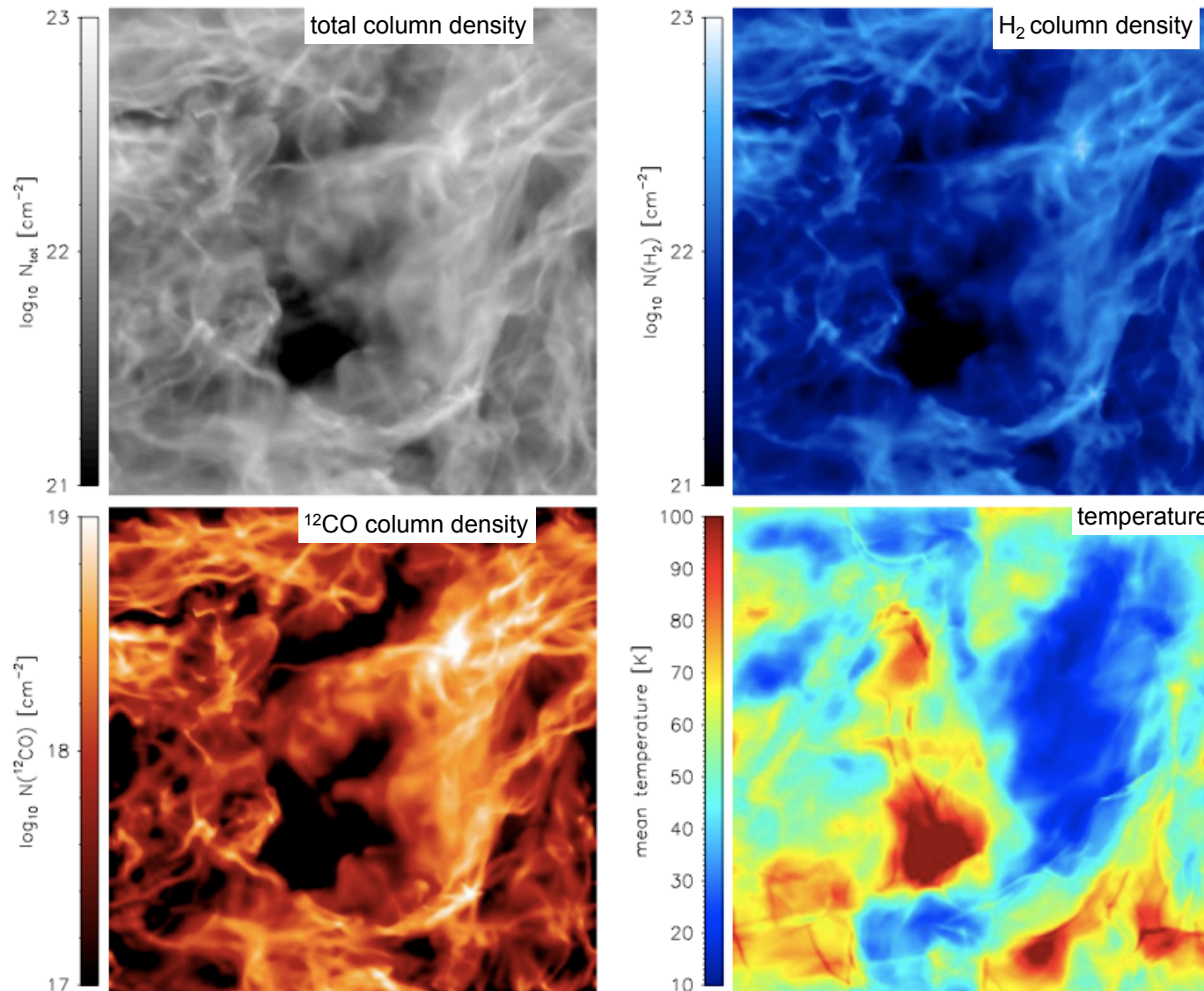


Figure 5. Time evolution of the mass-weighted abundances of atomic carbon (black lines), CO (red lines), and C⁺ (blue lines) in simulations with numerical resolutions of 64³ zones (dot-dashed), 128³ zones (dashed) and 256³ zones (solid).

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



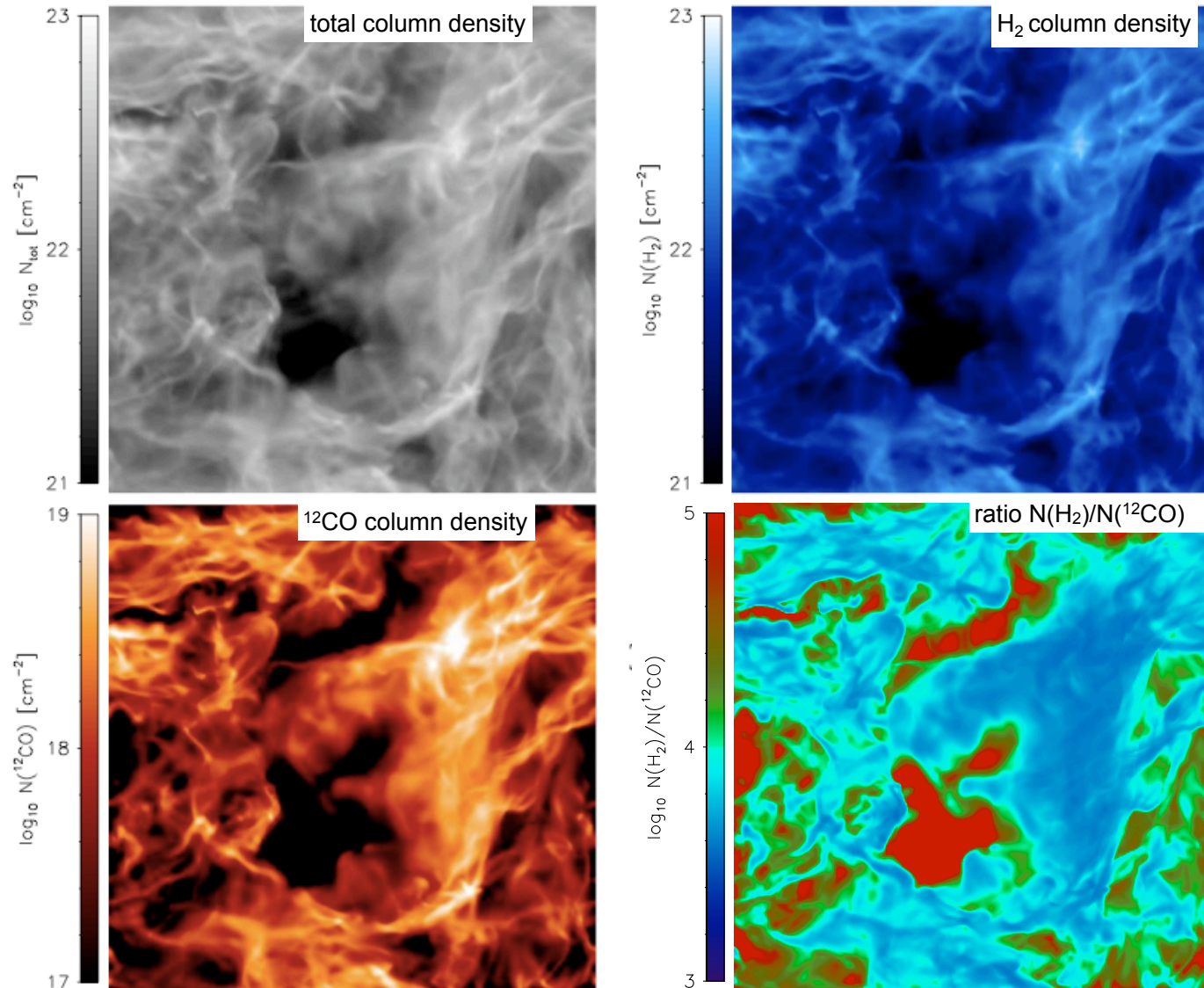
effects of chemistry 1



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



effects of chemistry 2



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

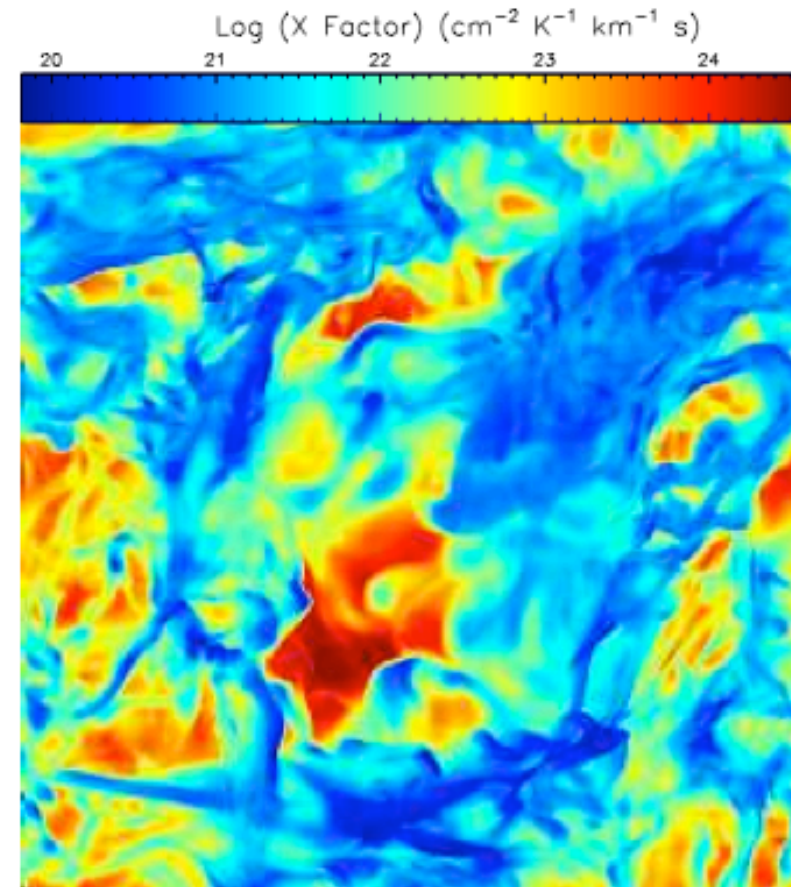
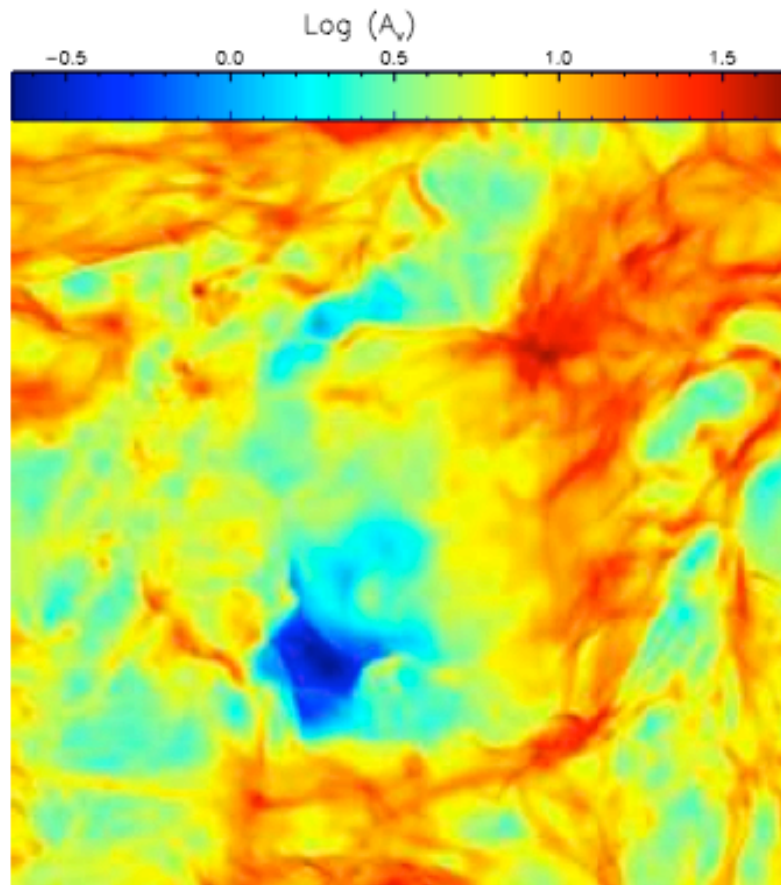


effects of chemistry 3

- deliverables / predictions:
 - x-factor estimates (as function of environmental conditions)
 - synthetic line emission maps (in combination with line transfer)
 - pdf's of density, velocity, emissivity / structure functions (to directly connect to observational regime)
 - **COMMENT:** density pdf is *NOT* lognormal!
--> implications for analytical IMF theories



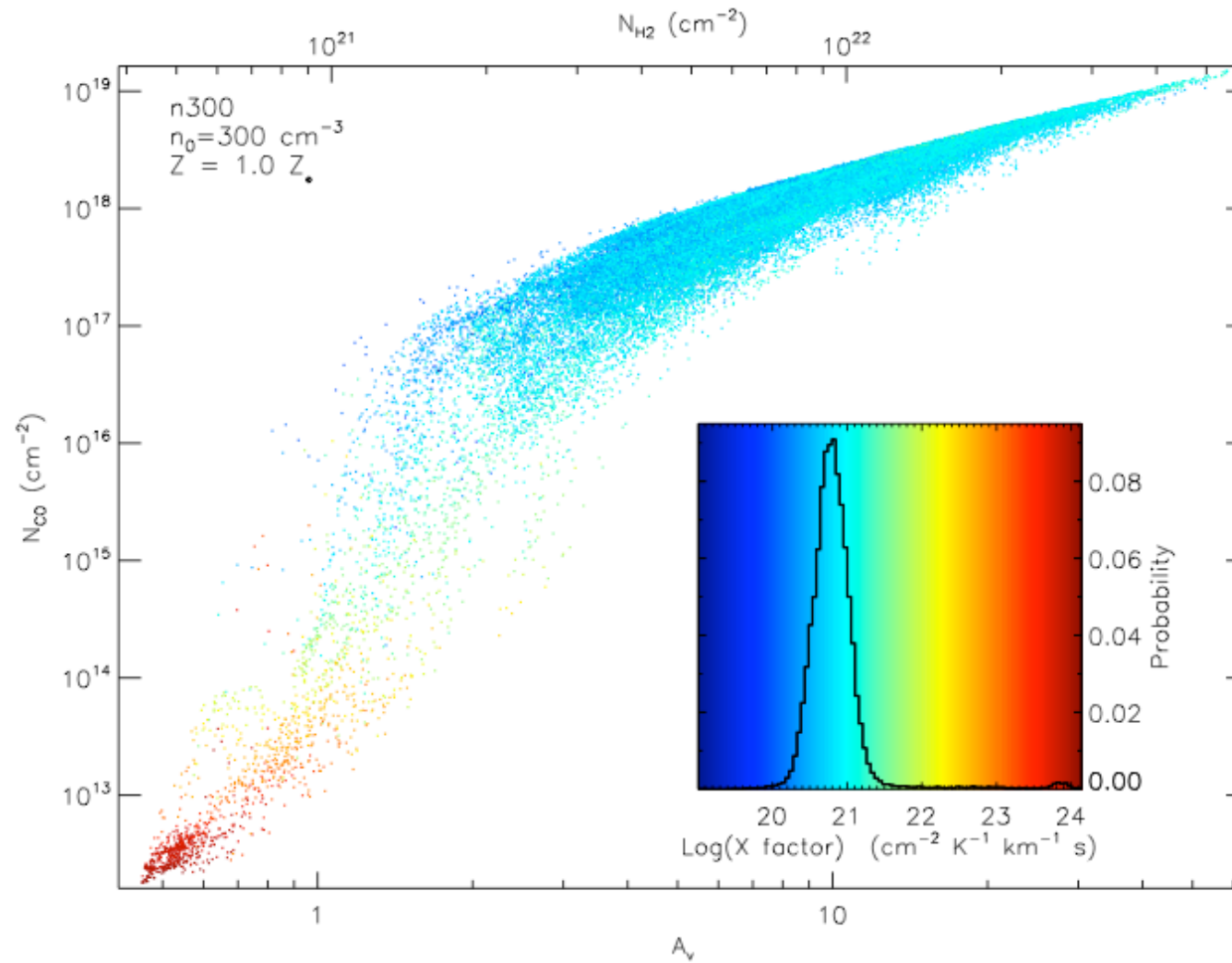
the x-factor



- Images of A_v (left) and the X factor (right) of model n300-Z03.



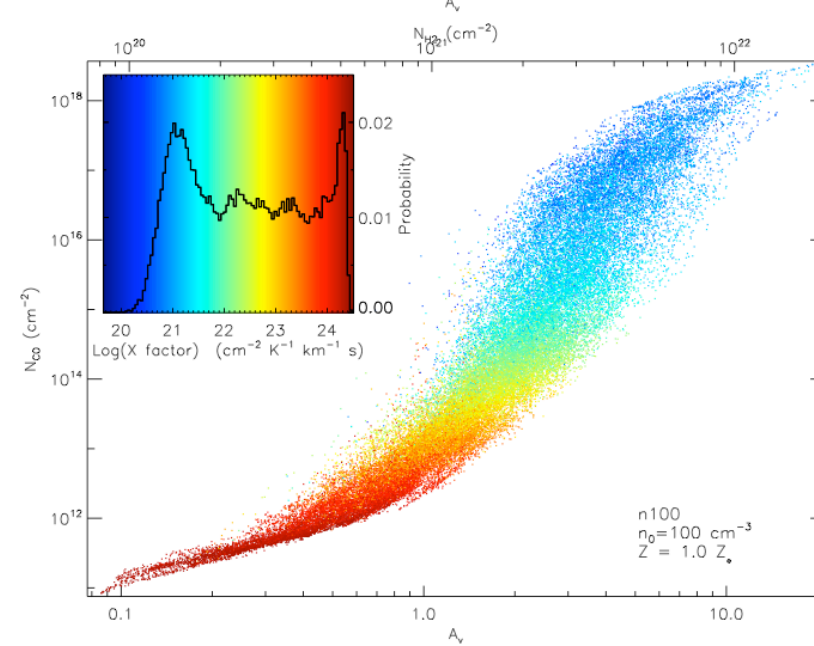
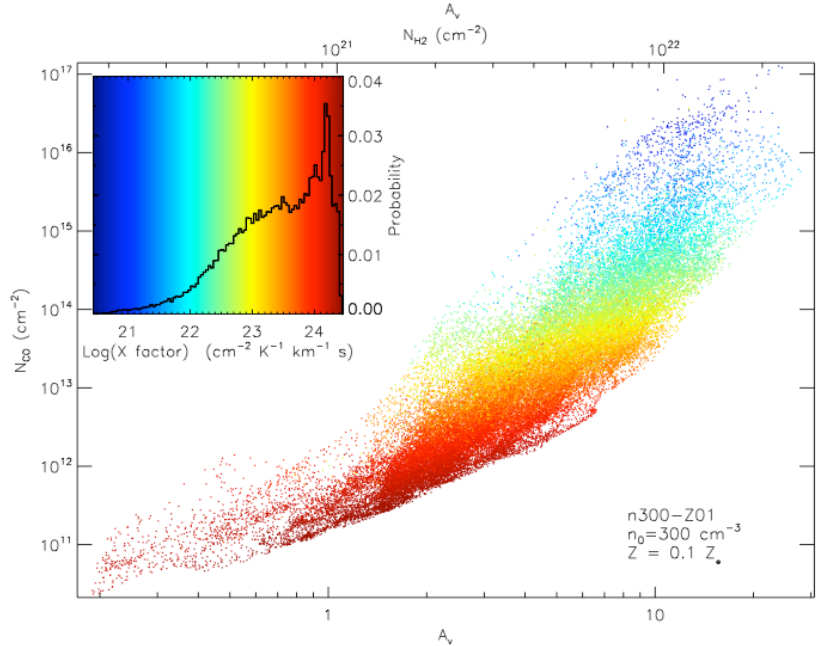
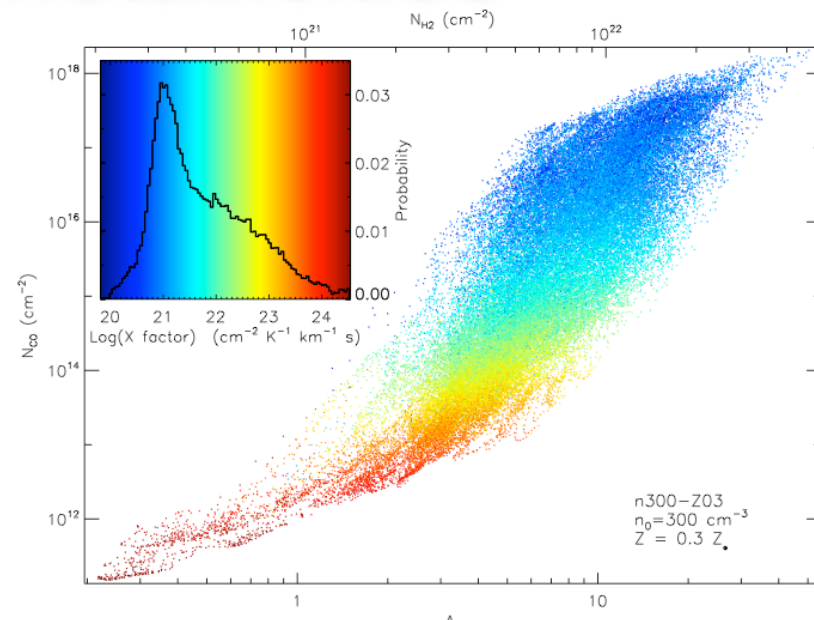
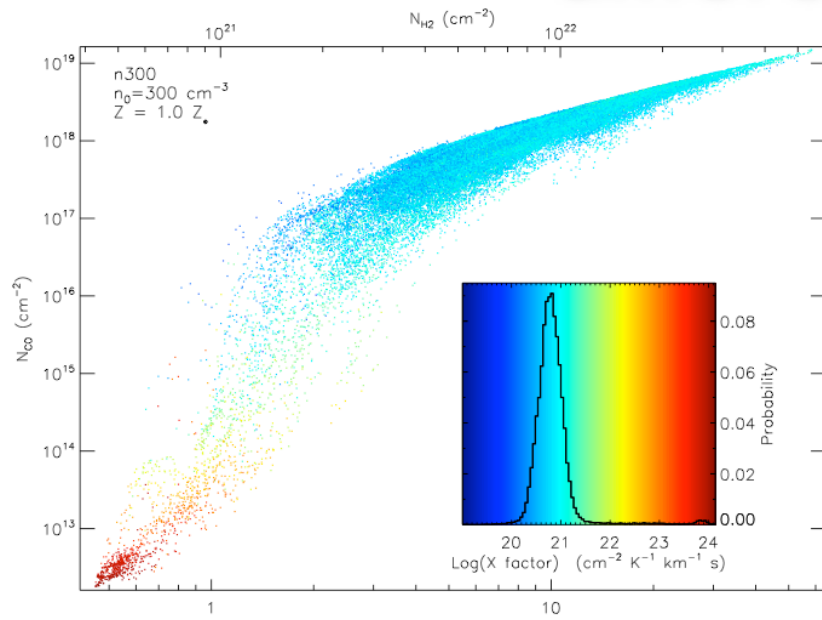
the x-factor



(Shetty, Glover, Dullemond, Klessen, in prep.)

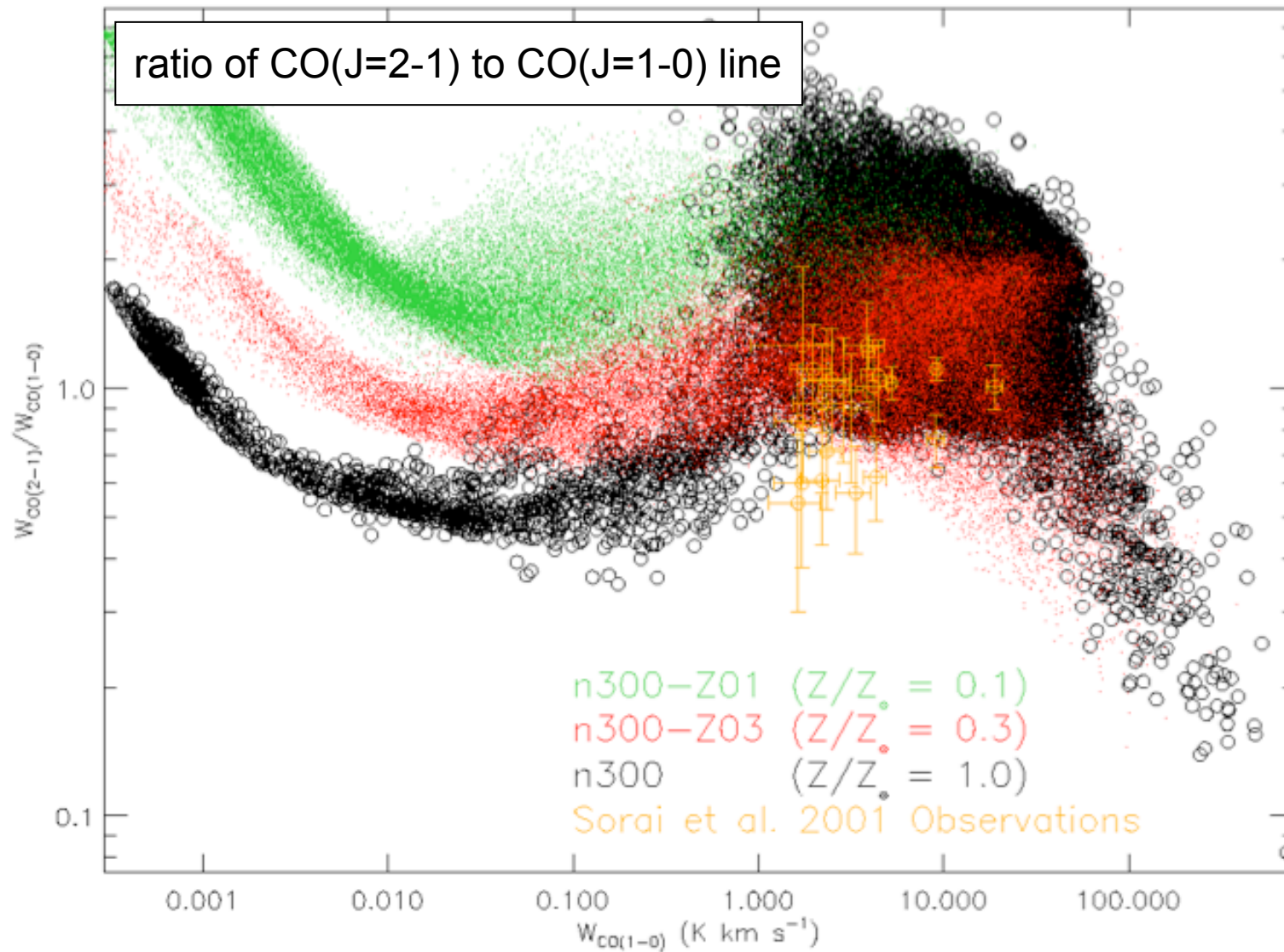


different metallicities





line ratios



(Shetty, Glover, Dullemond, Klessen, in prep.)



B-fields



how to make strong B-fields

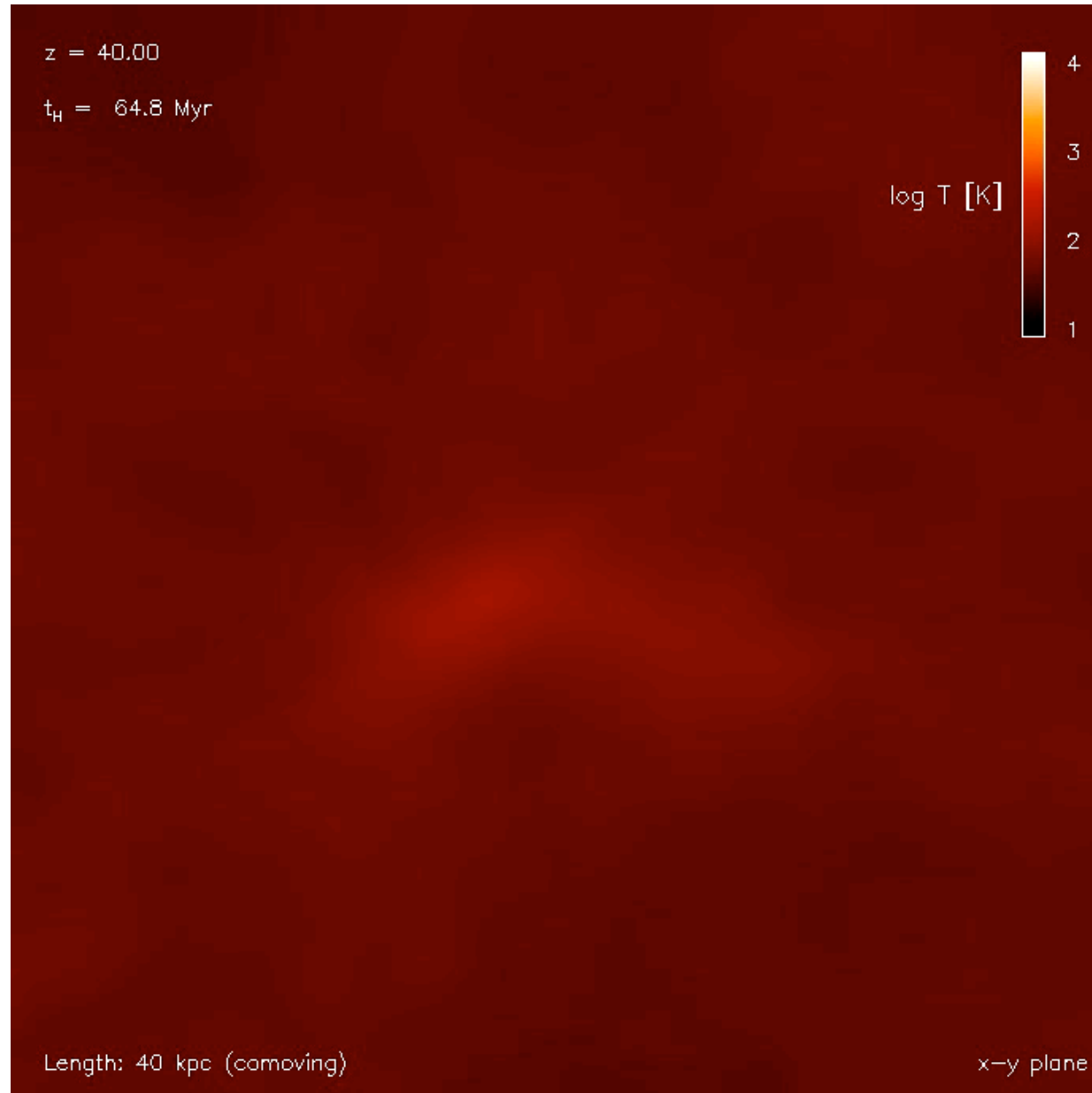
- we know the universe is magnetized (now)
- knowledge about B-fields in the high-redshift universe is extremely uncertain
 - inflation / QCD phase transition / Biermann battery / Weibel instability
- they are thought to be extremely small
- however, **THIS MAY BE WRONG!**



small-scale turbulent dynamo

- *idea*: the small-scale turbulent dynamo can generate strong magnetic fields from very small seed fields
- *approach*: model collapse of primordial gas ---> formation of the first stars in low-mass halo at redshift $z \sim 20$
- *method*: solve ideal MHD equations with very high resolution
 - grid-based AMR code FLASH
 - resolution up to 128^3 cells per Jeans volume (effective resolution 65536^3 cells)

turbulence developing in an atomic cooling halo

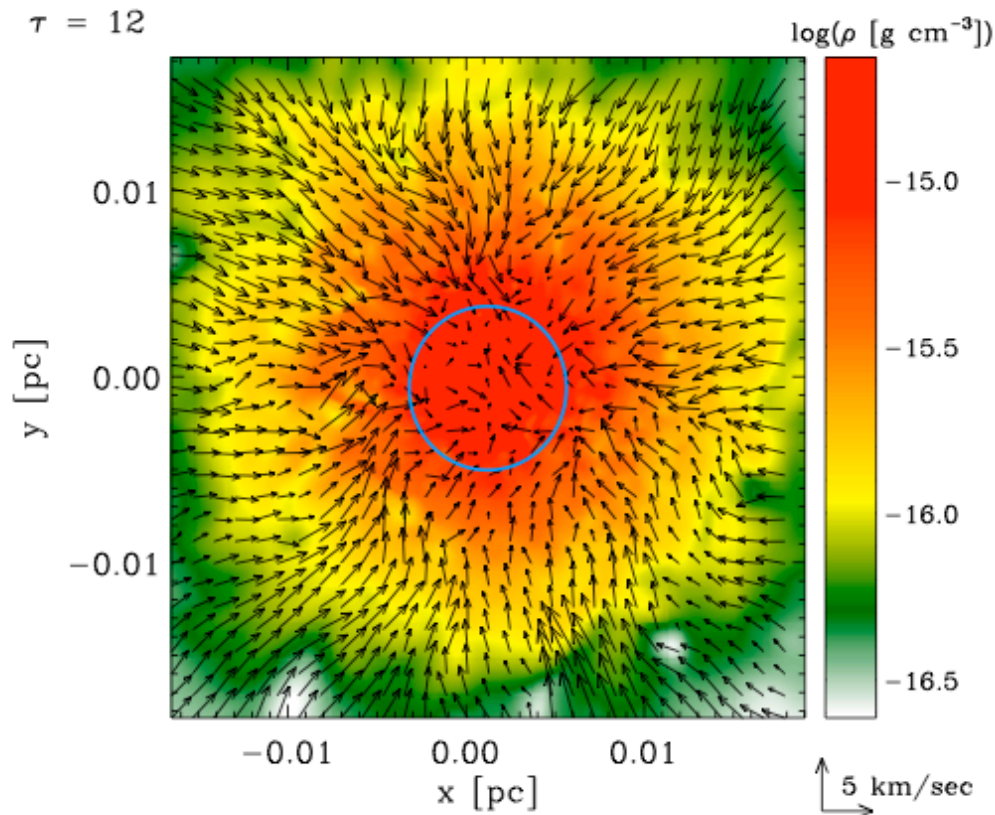


(Greif et al. 2008, MNRAS, 387, 1021, see also Wise & Abel 2007)

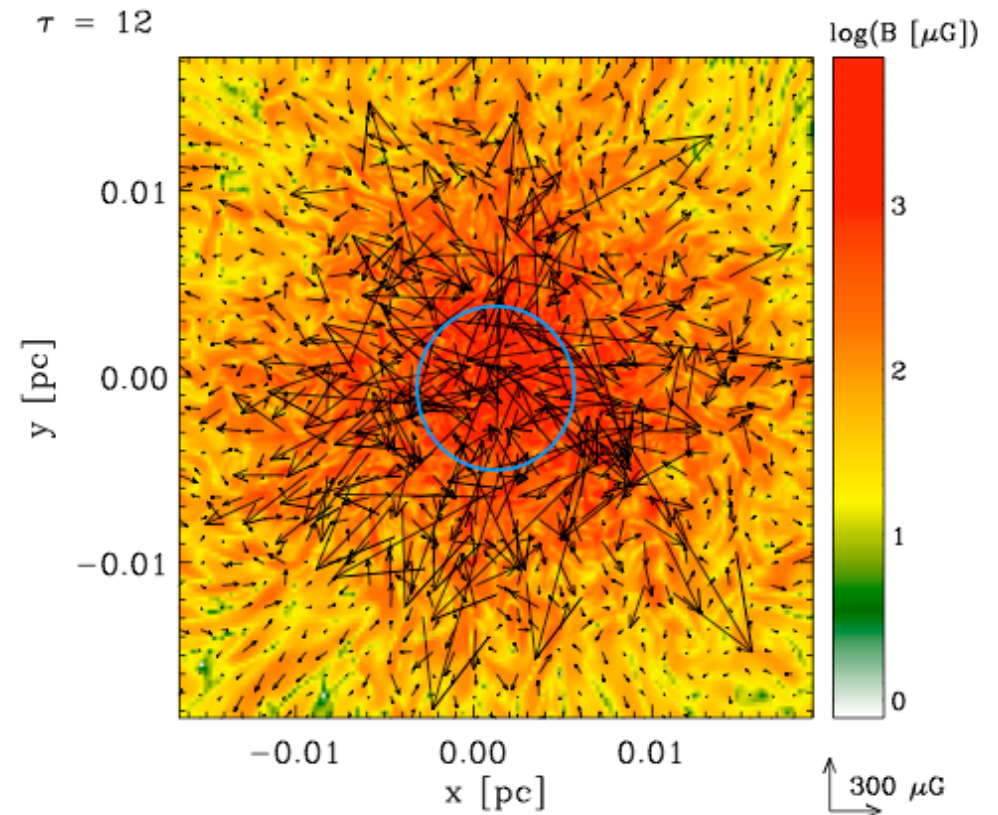
see also talk
by *Thomas Greif*



small-scale turbulent dynamo



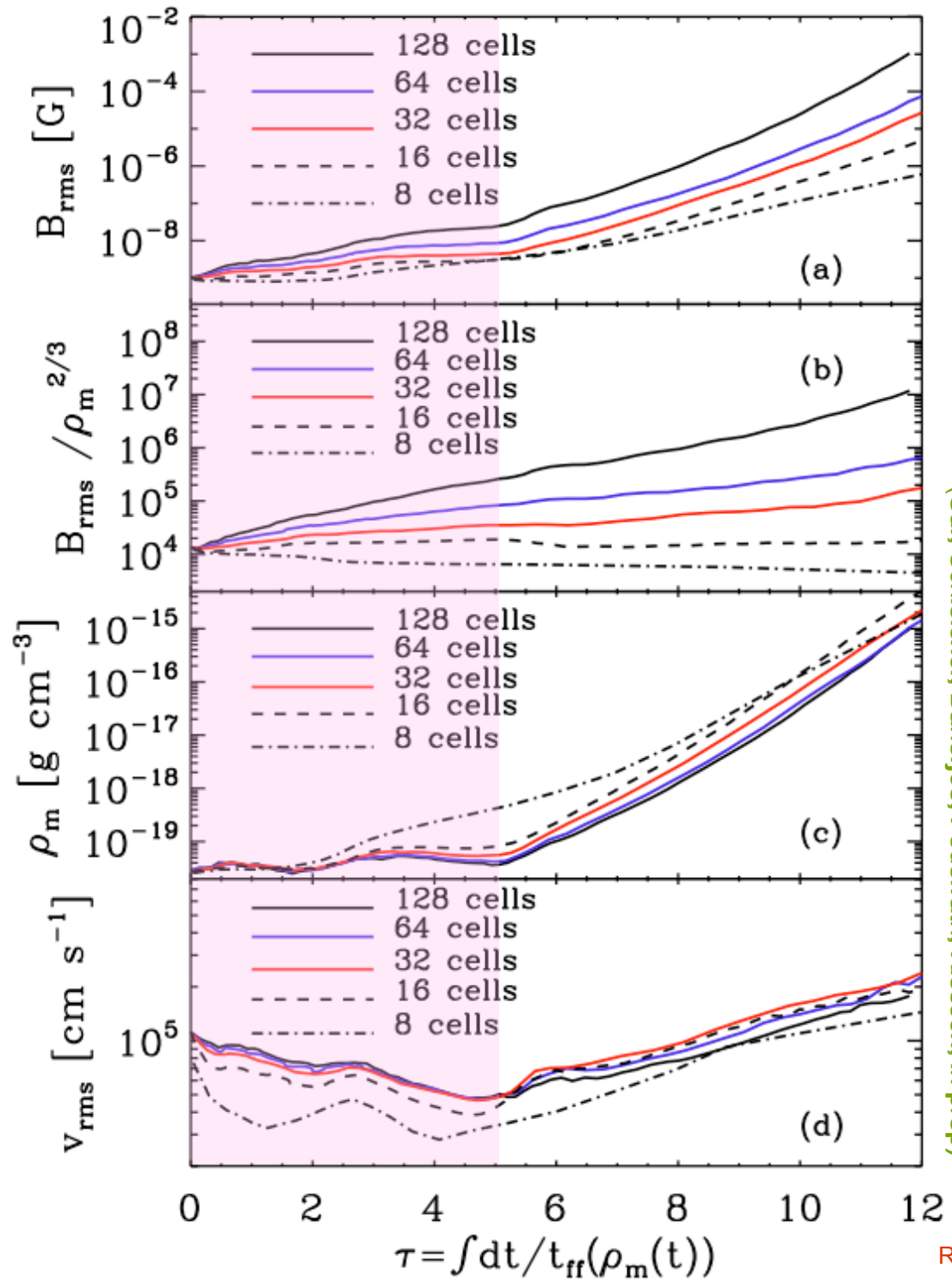
density, xy-velocity



B-field amplitude, xy-component



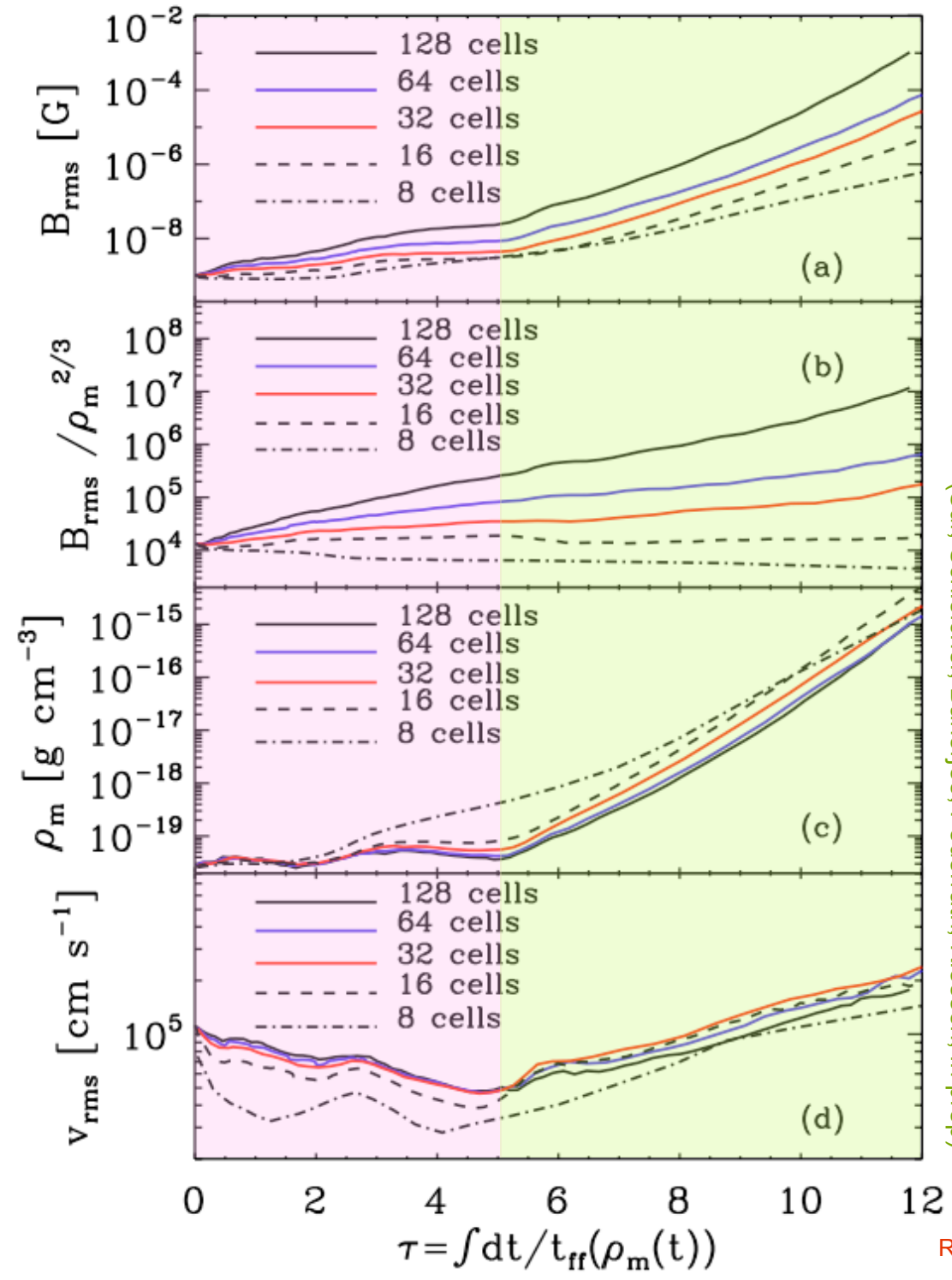
decay of turbulence



(Sur, Schleicher, Banerjee, Federrath, Klessen, in prep)



decay of turbulence

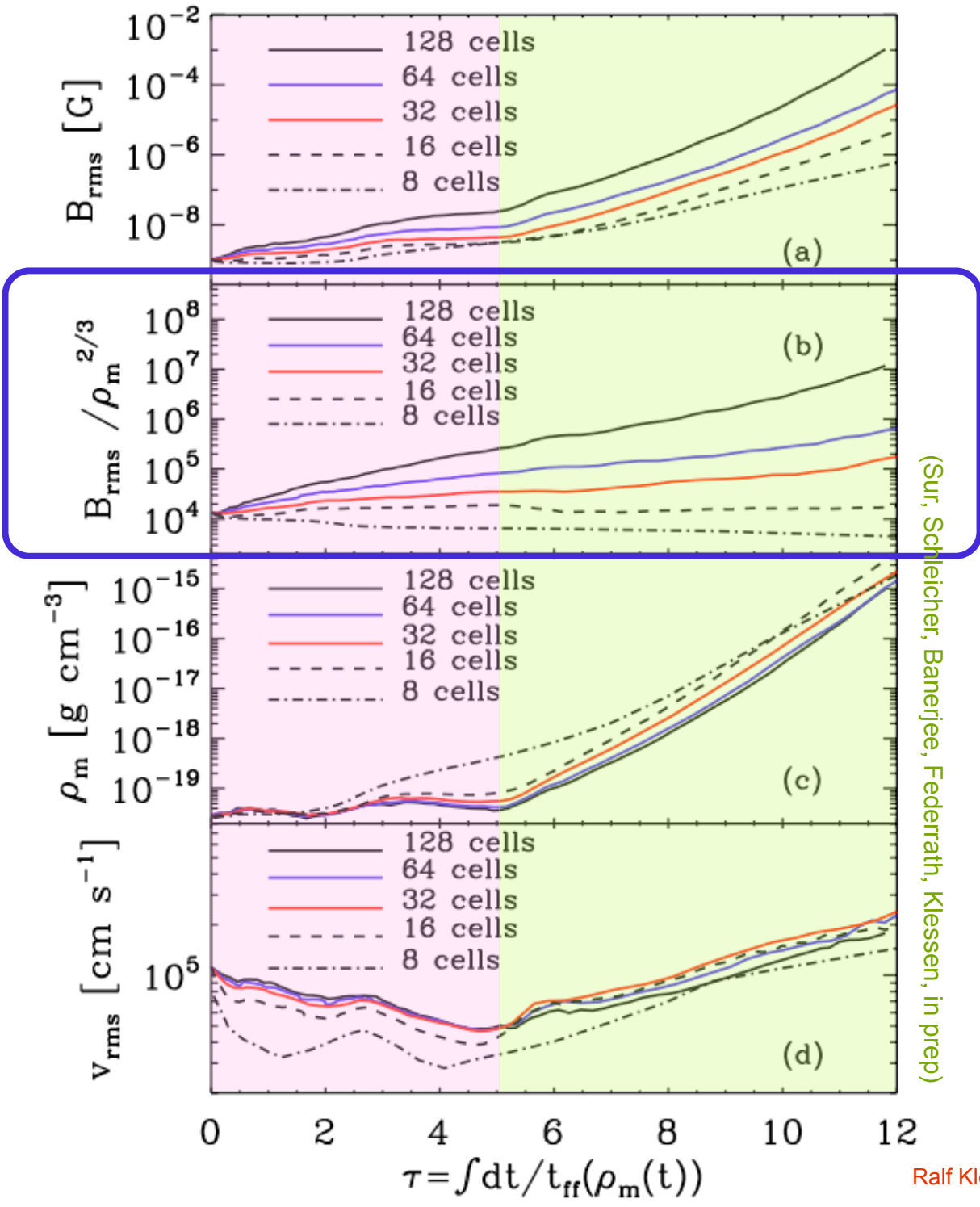


(Sur, Schleicher, Banerjee, Federrath, Klessen, in prep)

gravitational collapse,
accretion driven turbulence



decay of turbulence



gravitational collapse,
accretion driven turbulence



small-scale turbulent dynamo

- small-scale turbulent dynamo can generate dynamically significant B-fields in the during first star formation!
- expected saturation level $\sim 10\% - 20\%$ of equipartition value (Subramanian & Brandenburg 2005)
- needs very high resolution to be seen:

cells per Jeans length	max. refinement	max. effective resolution	min.cell size [cm]	mean growth rate Γ
8	10	4096	1.17×10^{16}	---
16	11	8192	5.86×10^{15}	0.021
32	12	16384	2.93×10^{15}	0.108
64	13	32768	1.46×10^{15}	0.188
128	14	65536	7.32×10^{14}	0.25



Summary



summary

- modeling ISM turbulence and star formation is feasible
 - more physics is needed (chemistry, radiation field, realistic sources of turbulence, etc.)
- caveat: all LES of ISM turbulence model “crude oil” not interstellar gas
- examples
 - statistical properties of the turbulence
 - molecular cloud formation
 - generation of the first dynamically significant magnetic fields in the universe



thanks