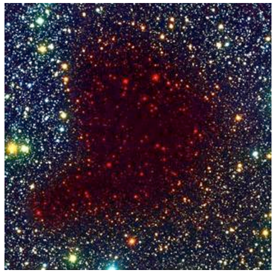
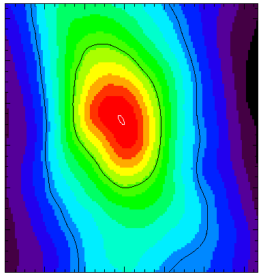
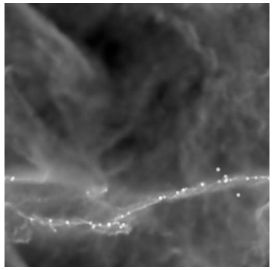
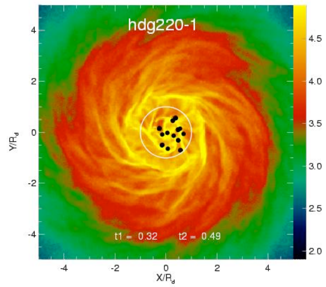
ISM Turbulence









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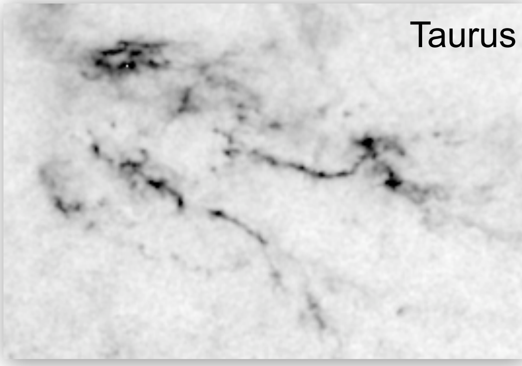
Agenda

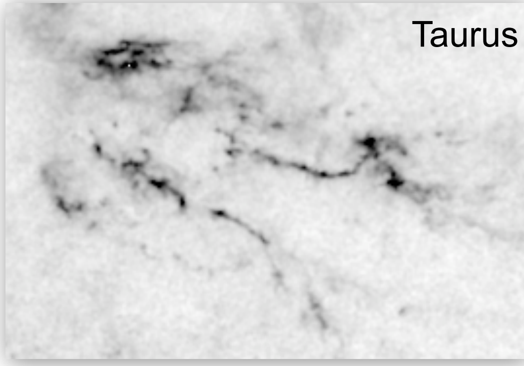
- some phenomenology
  - what we know
  - what we need to explain
- turbulence
  - some basic properties
  - formation of molecular clouds in galactic disks (H_2 & CO chemistry)
- summary: basic idea of gravoturbulent SF



Interstellar Matter: ISM

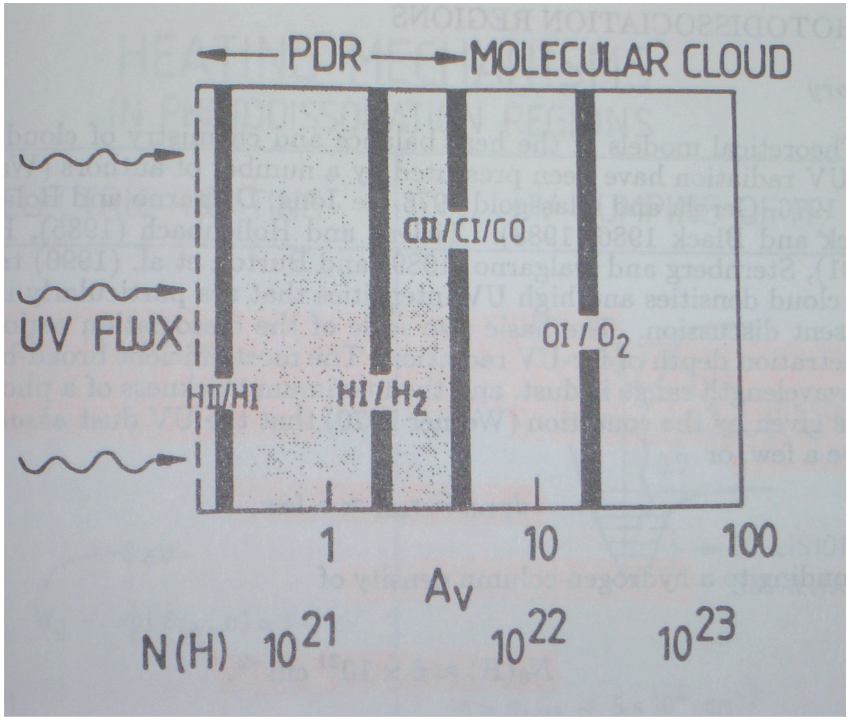
Abundances, scaled to 1.000.000 H atoms

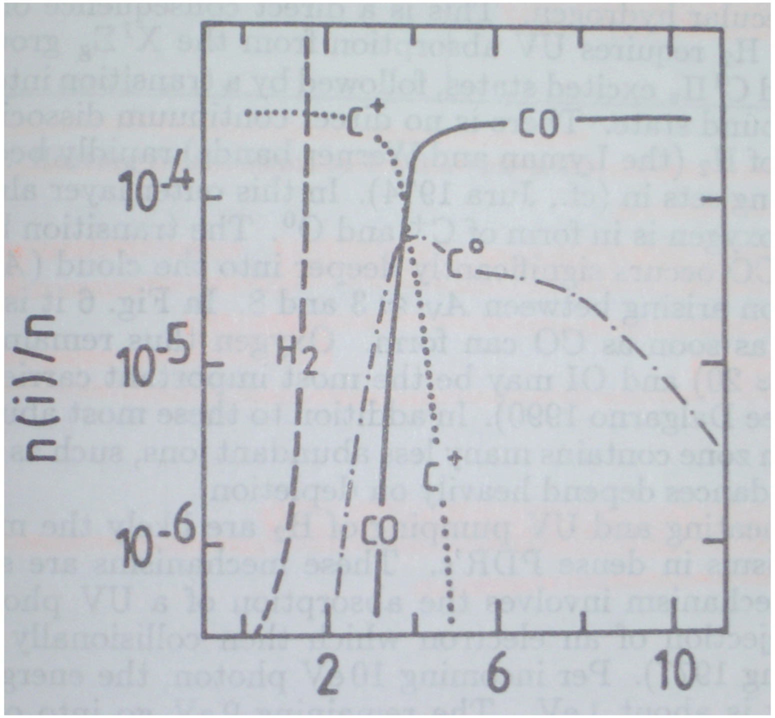
element		atomic number	abundance
Wasserstoff	H	1	1.000.000
Deuterium	$_1H^2$	1	16
Helium	He	2	68.000
Kohlenstoff	C	6	420
Stickstoff	N	7	90
Sauerstoff	O	8	700
Neon	Ne	10	100
Natrium	Na	11	2
Magnesium	Mg	12	40
Aluminium	Al	13	3
Silicium	Si	14	38
Schwefel	S	16	20
Calcium	Ca	20	2
Eisen	Fe	26	34
Nickel	Ni	28	2



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

Phases of the ISM





A_V

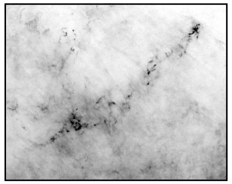
HII HI H_2

Dichte- / Säulendichte nimmt zu

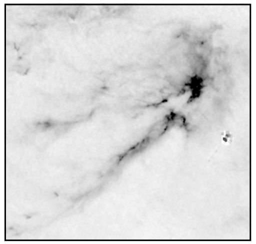
A_V bezeichnet die Extinktion, dh. die Abschwächung der einfallenden Strahlung.

nearby molecular clouds

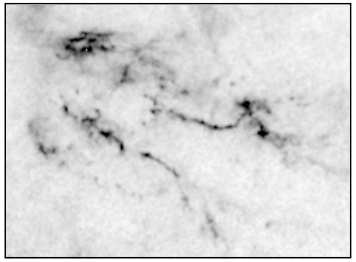
-Pipe



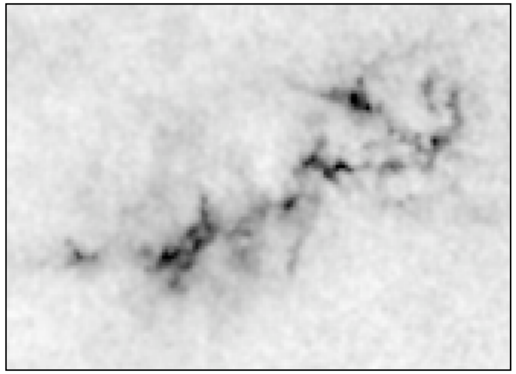
-Ophiuchus



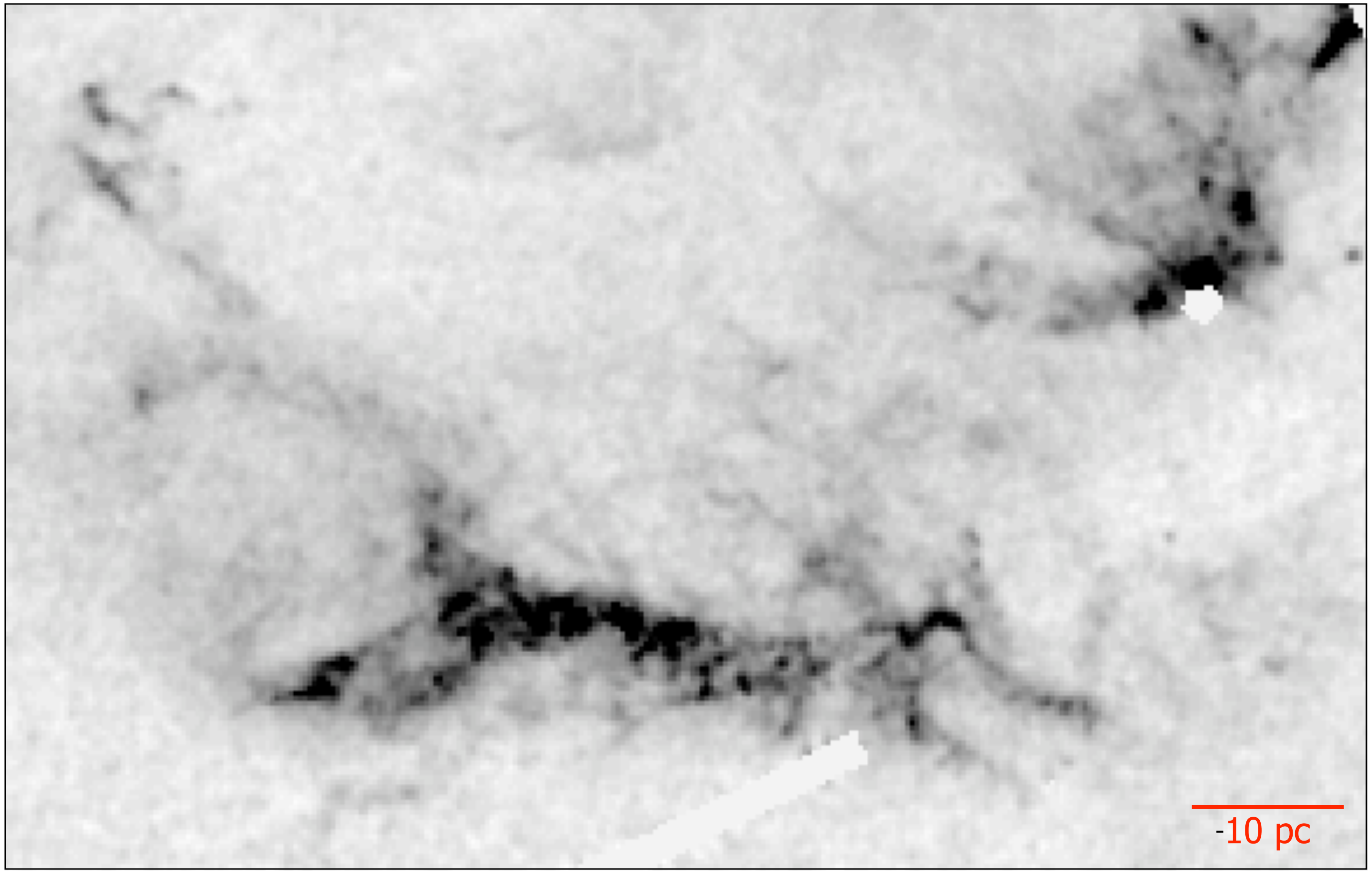
-Taurus



-Perseus



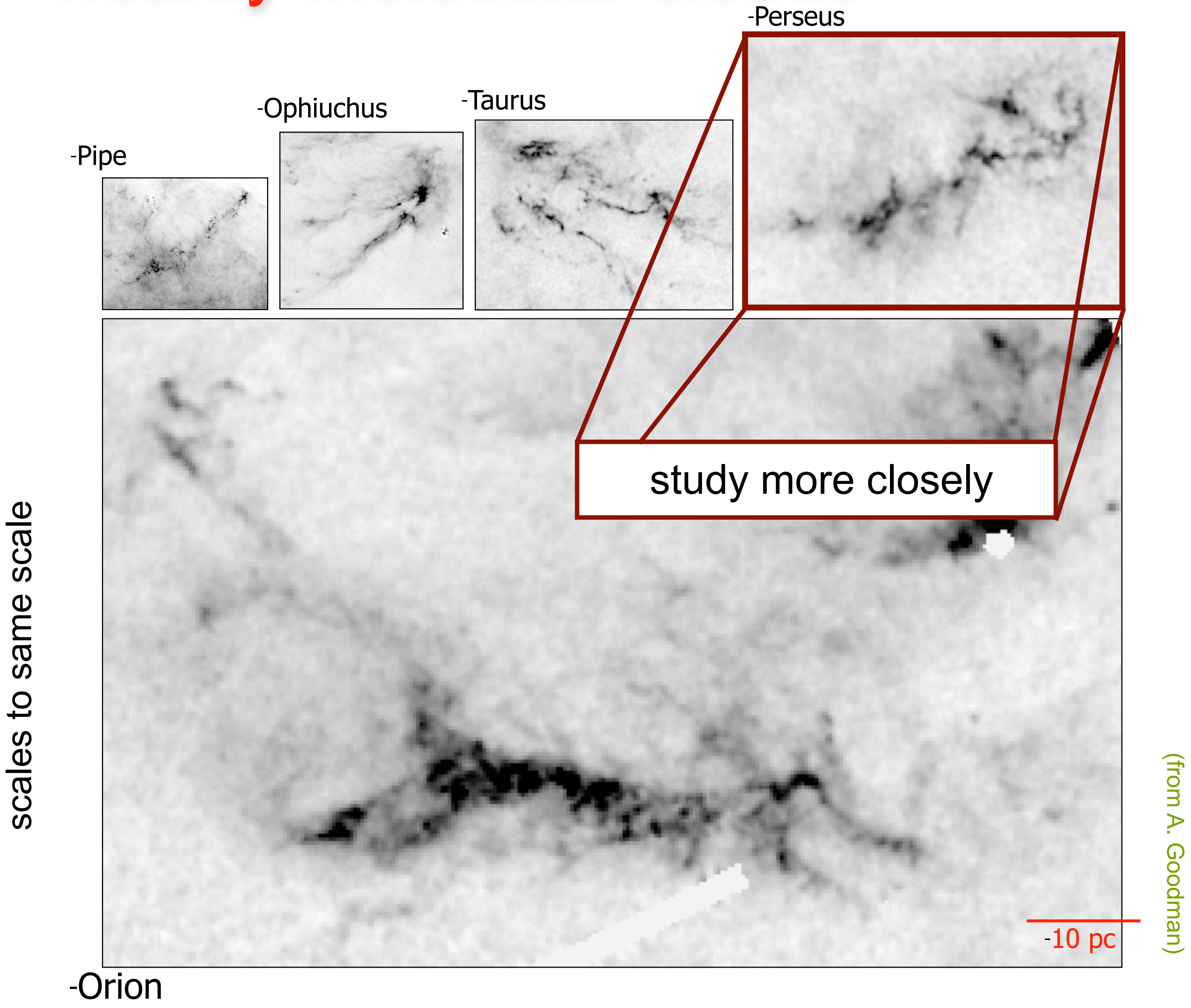
scales to same scale

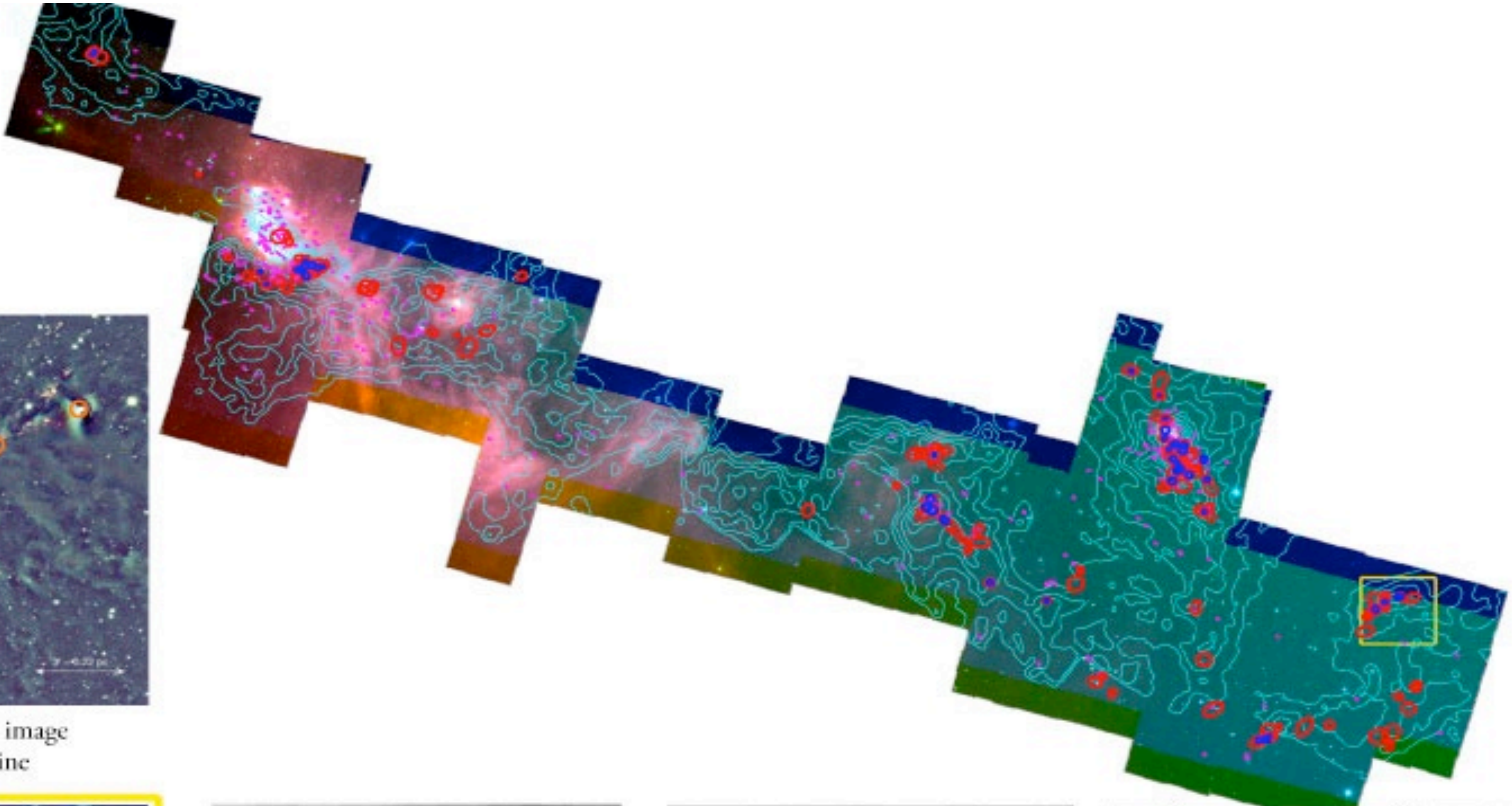


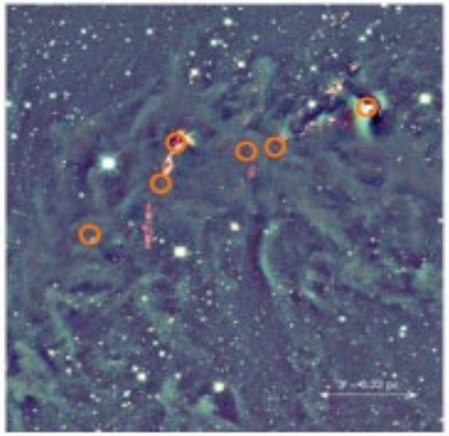
-Orion

(from A. Goodman)

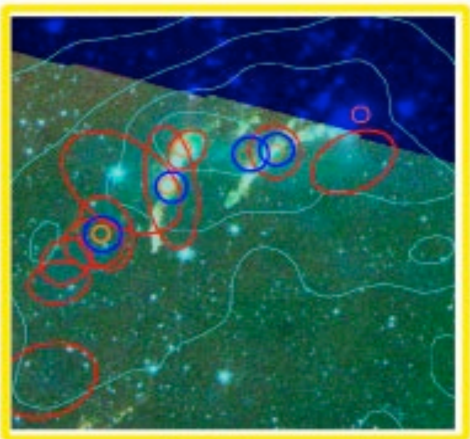
nearby molecular clouds



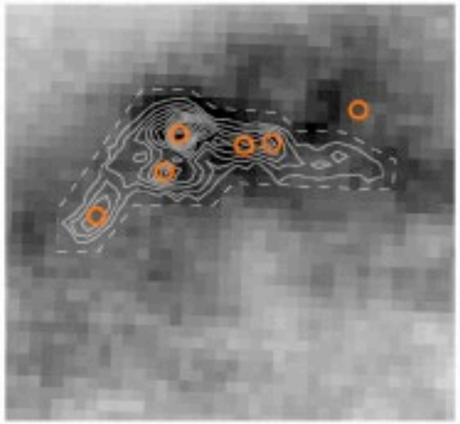




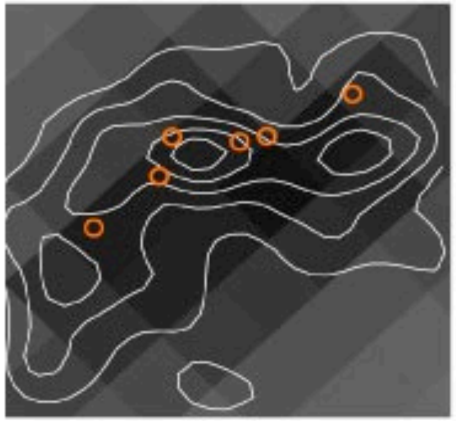
J,H,K Near-IR image of Cloudshine



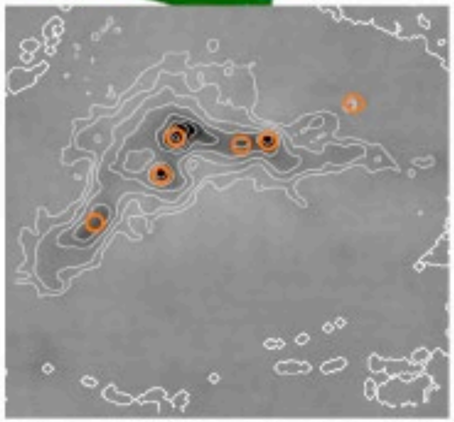
850 micron and 1.1 mm clumps on a c2d IRAC 3-color image



N_2H^+ on ^{13}CO integrated intensity



Deep NIR Extinction on 2MASS Extinction



1.2 mm (IRAM) on 850 micron (SCUBA) continuum

images from Alyssa Goodman

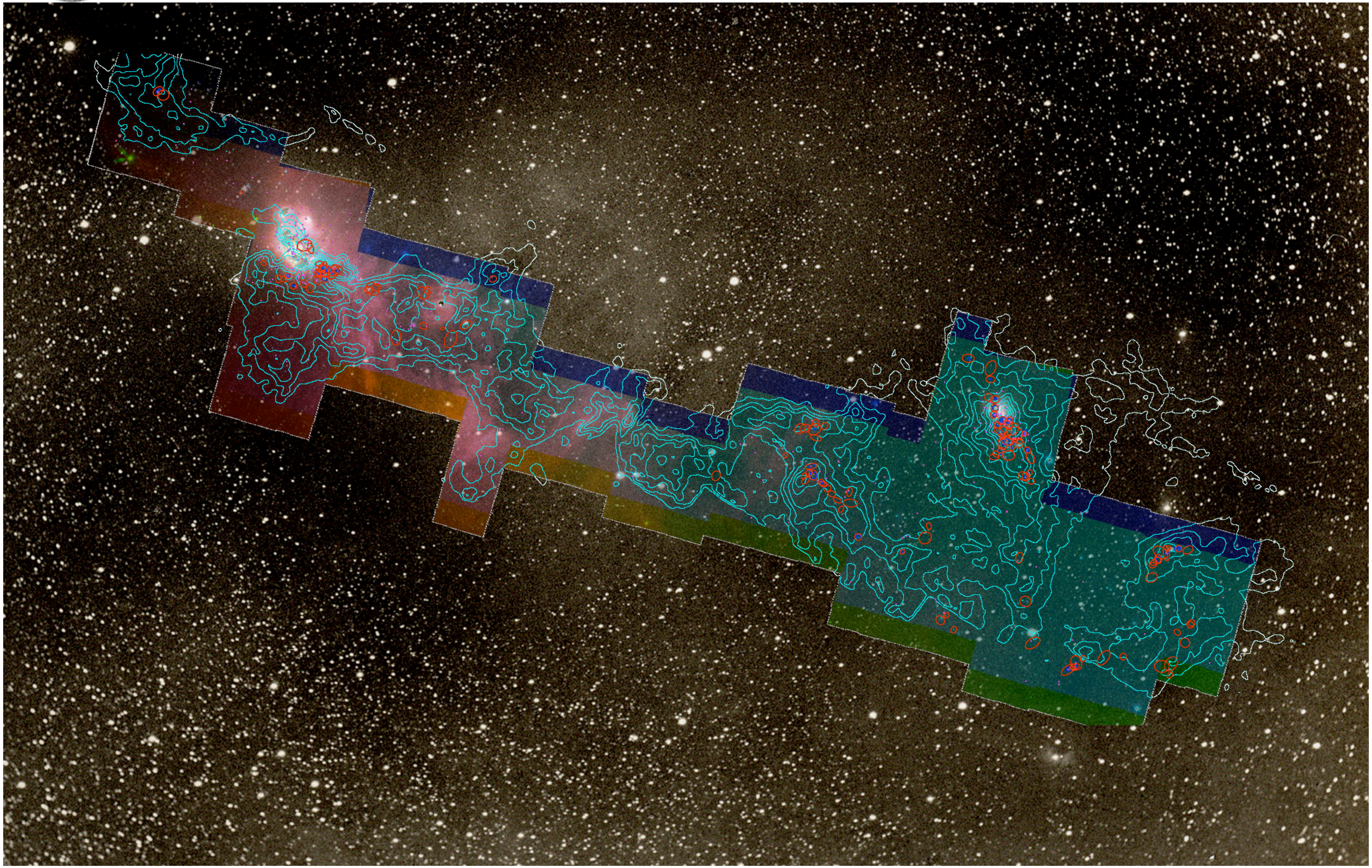
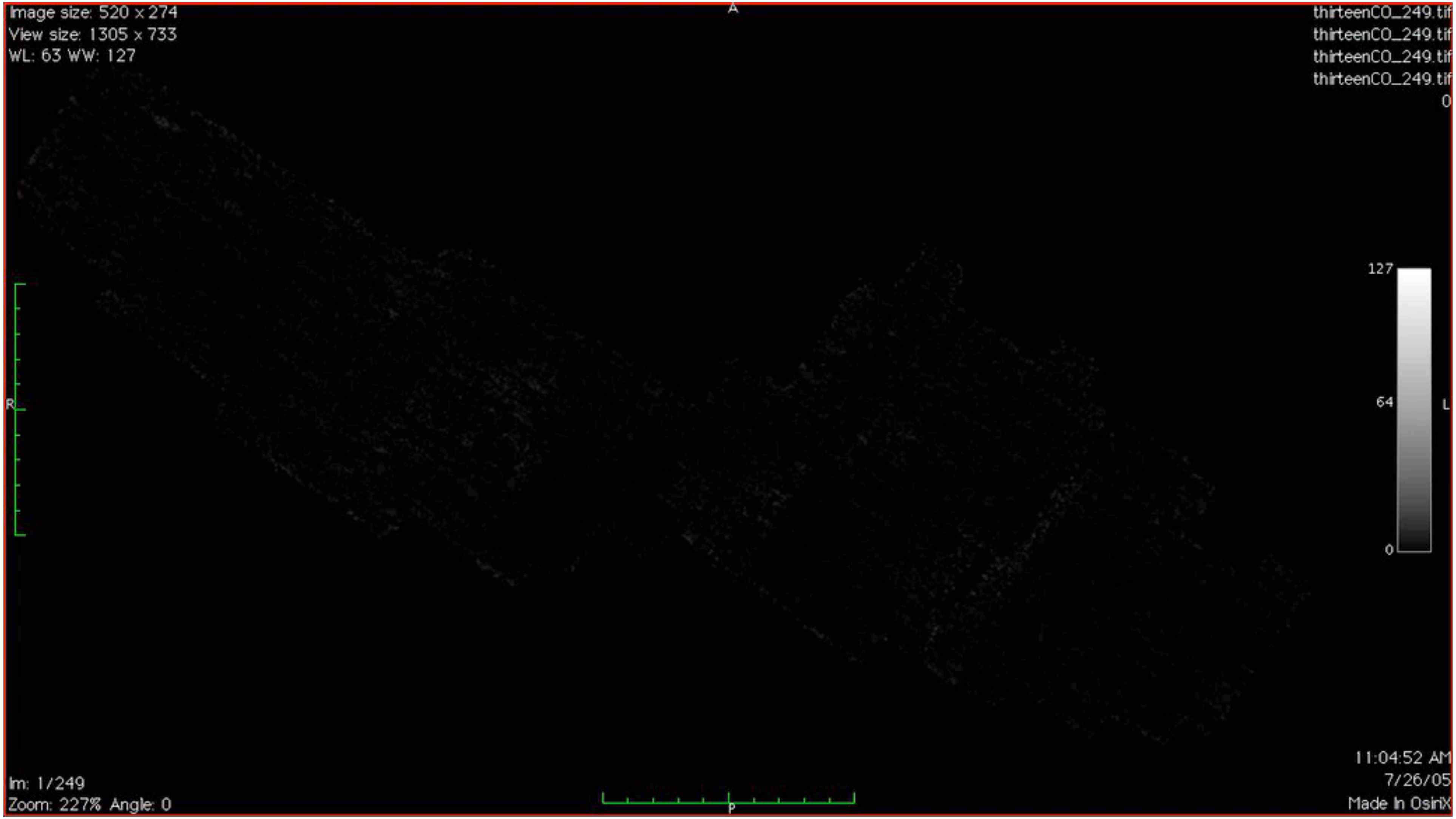


image from Alyssa Goodman: COMPLETE survey



velocity distribution in Perseus

velocity cube from Alyssa Goodman: COMPLETE survey

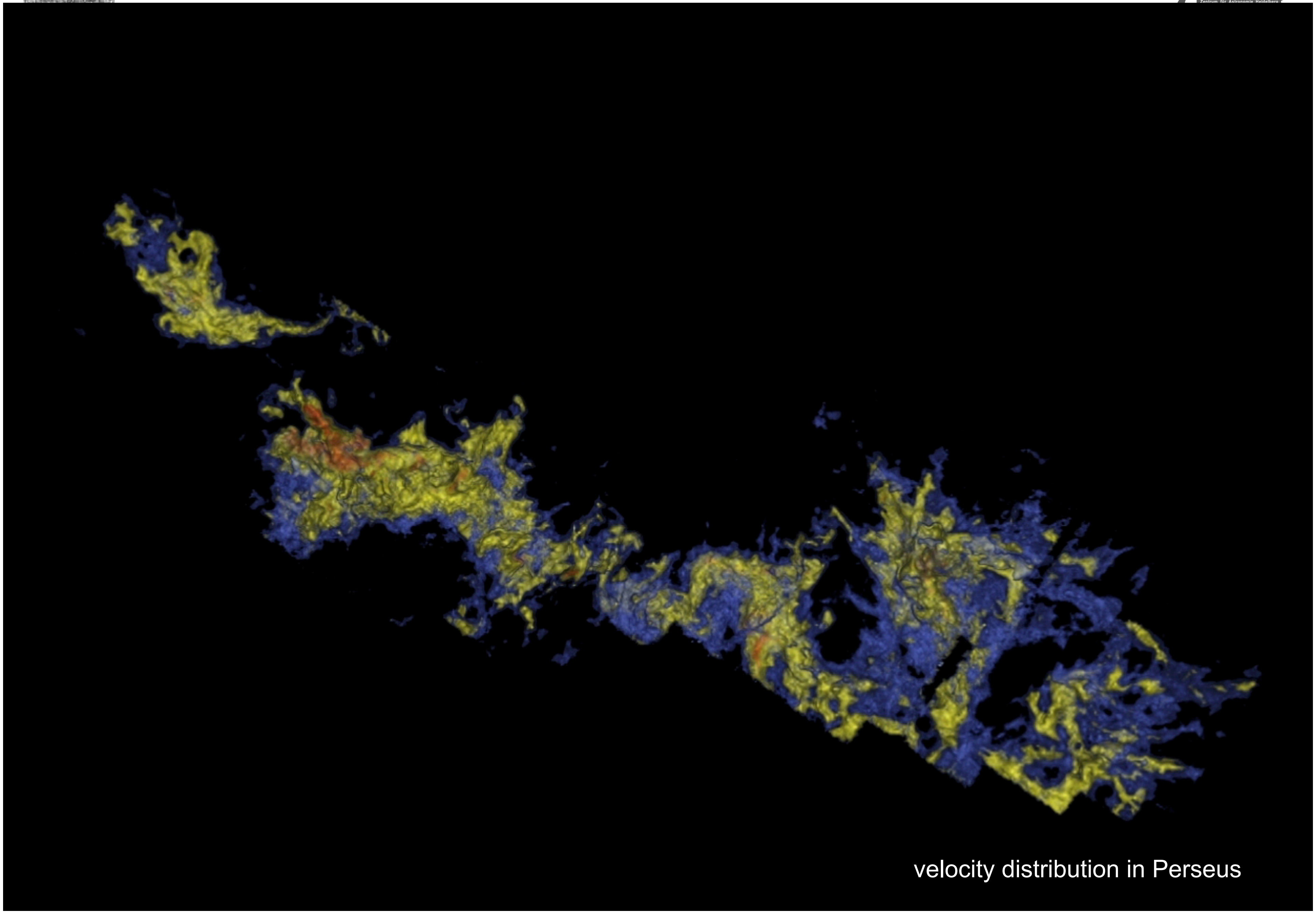


image from Alyssa Goodman: COMPLETE survey

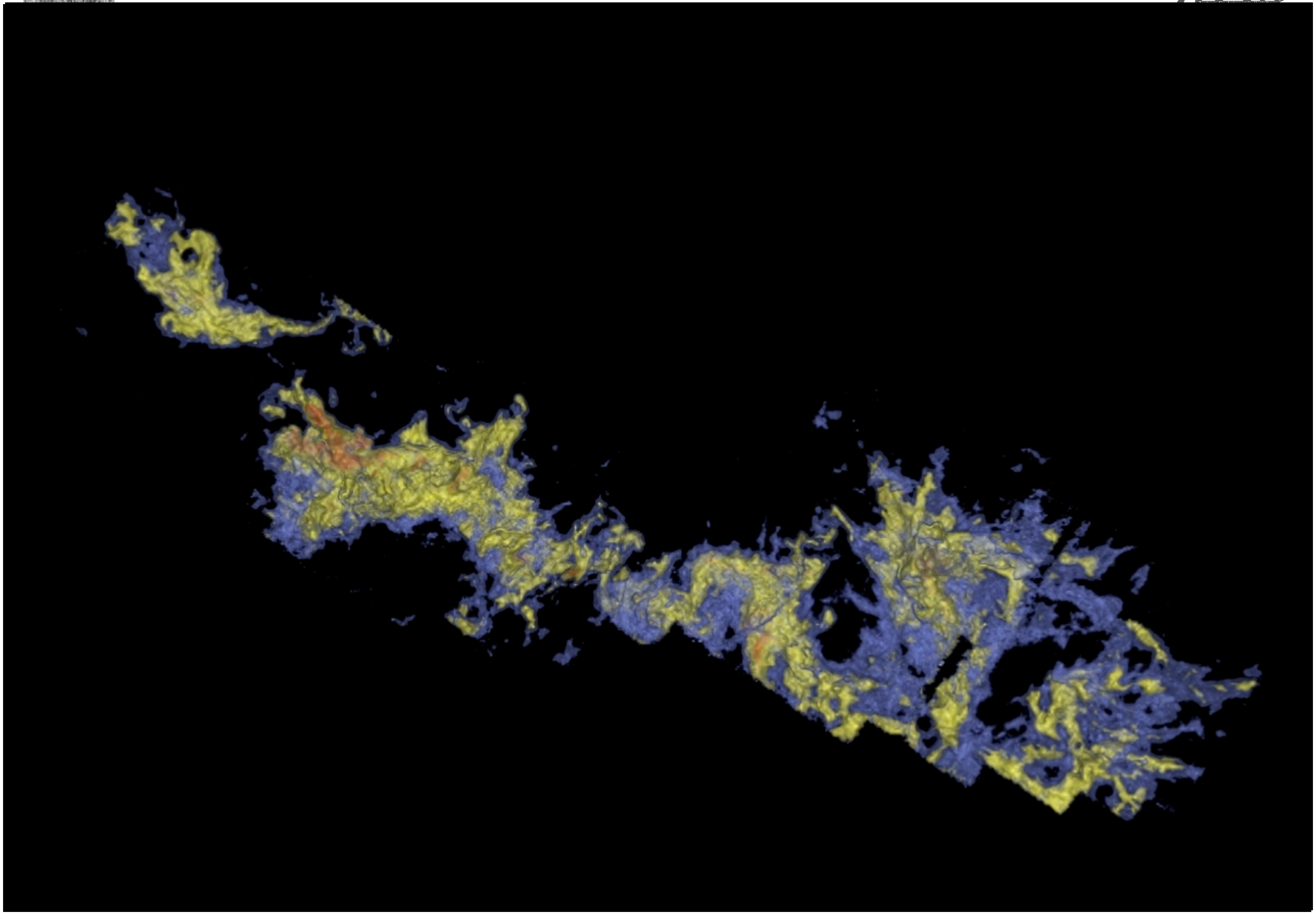
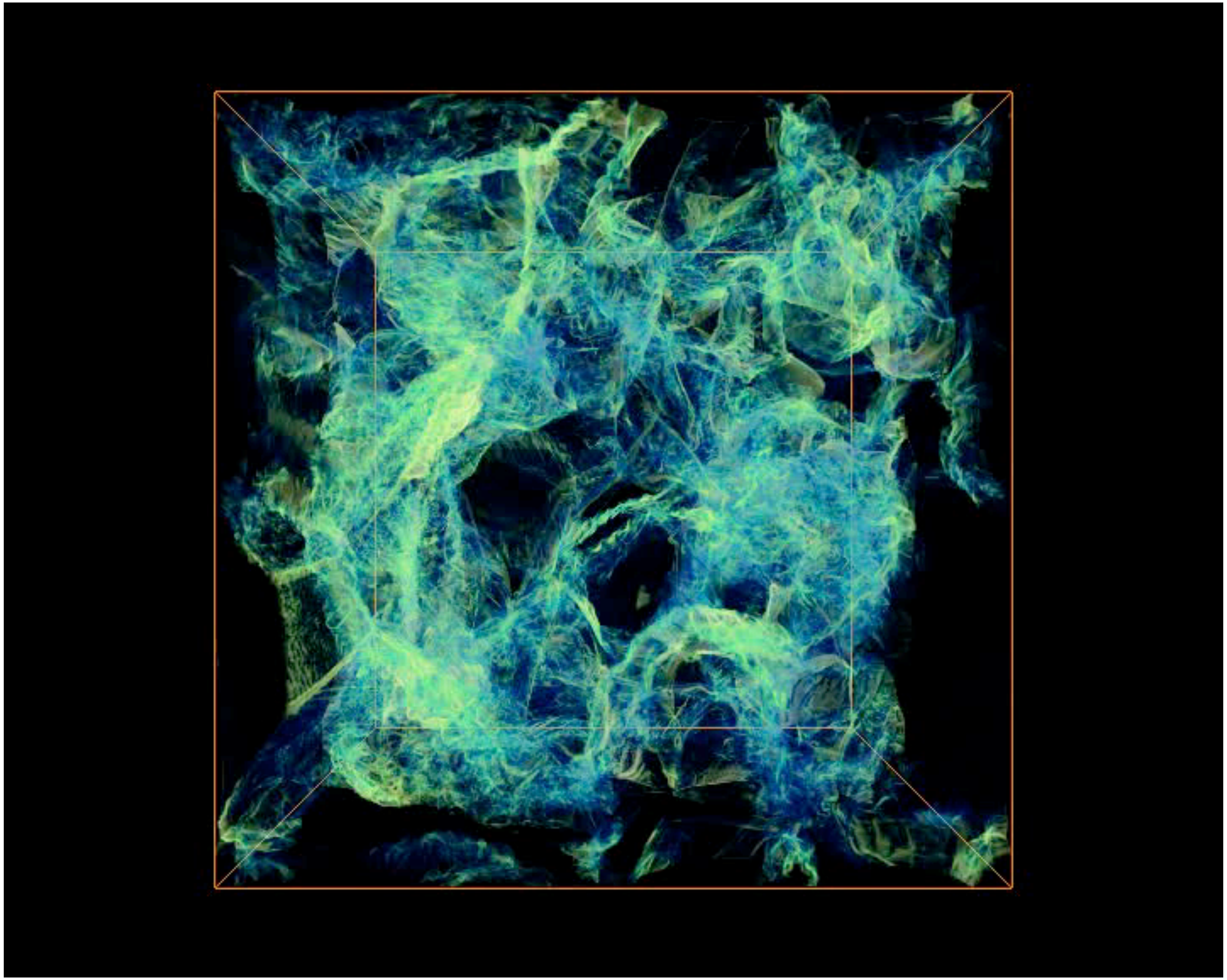
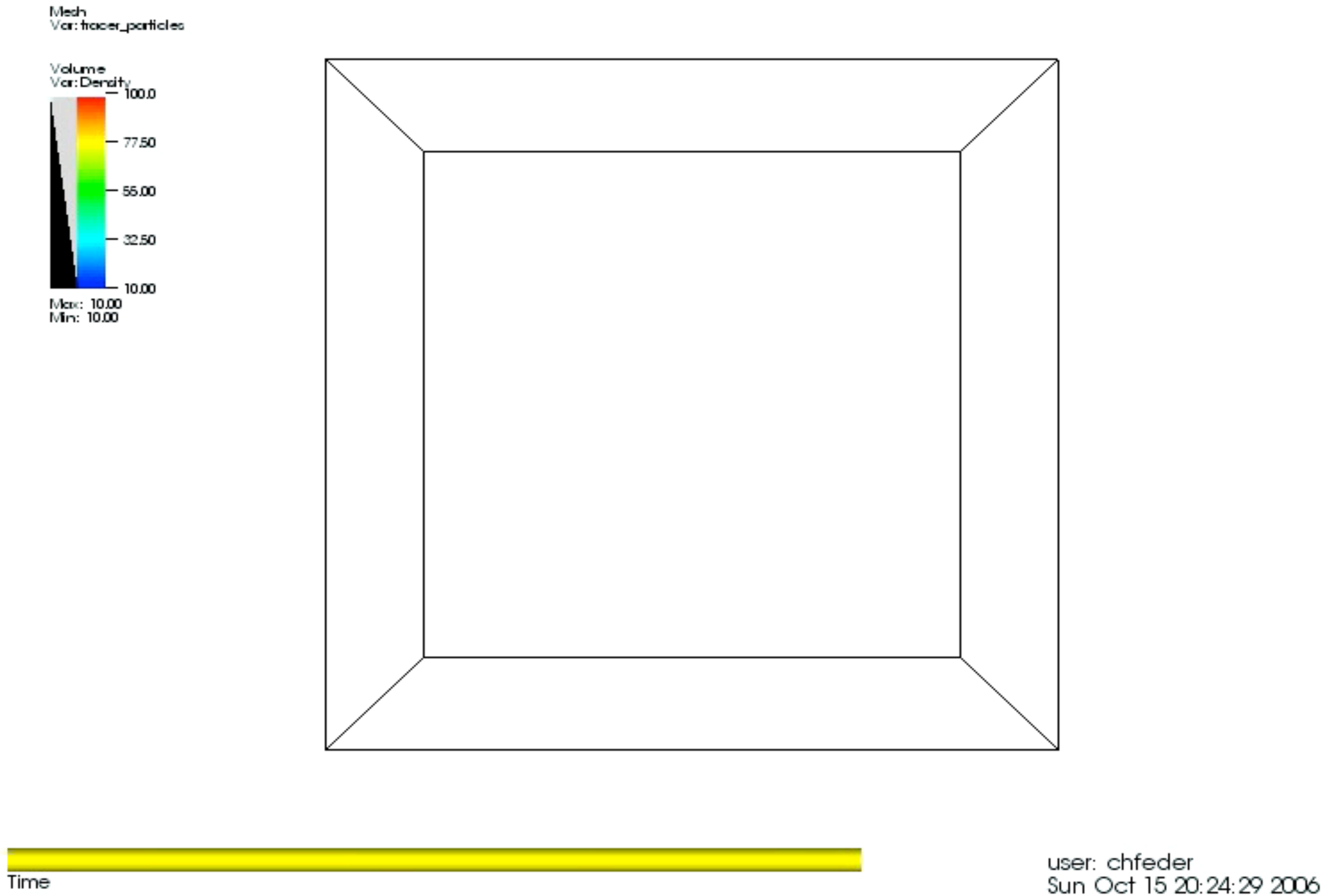


image from Alyssa Goodman: COMPLETE survey



(movie from Christoph Federrath)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Volume
Var: Density
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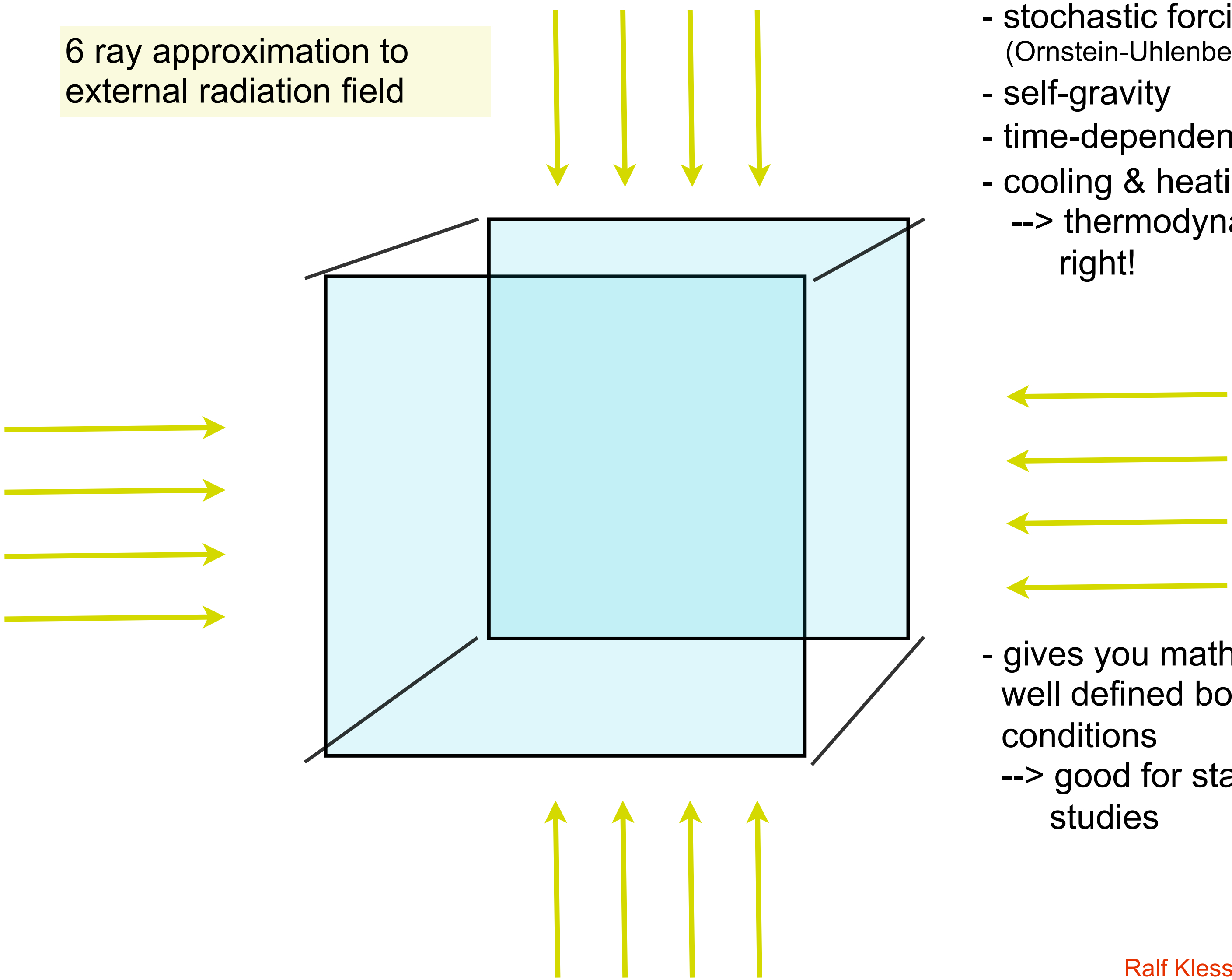
77.50
55.00
32.50
10.00
Max: 10.00
Min: 10.00
Time
user: chfeder
Sun Oct 15 20:24:29 2006

experimental set-up

- AMR MHD (B = 2 muG)
- stochastic forcing
  (Ornstein-Uhlenbeck)
- self-gravity
- time-dependent chemistry
- cooling & heating processes
  --> thermodynamics done right!



- gives you mathematically well defined boundary conditions
  --> good for statistical studies

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

(Glover, Federrath, Mac Low, Klessen, in prep)

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, in prep)

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	$H + e^- \rightarrow H^- + \gamma$	$k_1 =$ [illegible] $= dex[-16.420 + 0.1998(\log T)^2$ $- 5.447 \times 10^{-3}(\log T)^4$ $+ 4.0415 \times 10^{-5}(\log T)^6]$	[illegible] $T > 6000$ K	1
2	$H^- + H \rightarrow H_2 + e^-$	$k_2 = 1.5 \times 10^{-9}$ $= 4.0 \times 10^{-9} T^{-0.17}$	$T \leqslant 300$ K $T > 300$ K	2
3	$H + H^+ \rightarrow H_2^+ + \gamma$	$k_3 = dex[-19.38 - 1.523 \log T$ $+ 1.118(\log T)^2 - 0.1269(\log T)^3]$		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	$H_2^+ + e^- \rightarrow H + H$	$k_6 = 1.0 \times 10^{-8}$ $= 1.32 \times 10^{-6} T^{-0.76}$	$T \leqslant 617$ 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	$H_2 + H \rightarrow H + H + H$	$k_{9,l} = 6.67 \times 10^{-12} T^{1/2} \exp\left[-(1 + \frac{63590}{T})\right]$ $k_{9,h} = 3.52 \times 10^{-9} \exp\left(-\frac{43900}{T}\right)$ $n_{cr,H} = dex\left[3.0 - 0.416 \log\left(\frac{T}{10000}\right) - 0.327\left\{\log\left(\frac{T}{10000}\right)\right\}^2\right]$		9 10 10
10	$H_2 + H_2 \rightarrow H_2 + H + H$	$k_{10,l} = \frac{5.996 \times 10^{-30} T^{4.1881}}{(1.0 + 6.761 \times 10^{-6} T)^{5.6881}} \exp\left(-\frac{54657.4}{T}\right)$ $k_{10,h} = 1.3 \times 10^{-9} \exp\left(-\frac{53300}{T}\right)$ $n_{cr,H_2} = dex\left[4.845 - 1.3 \log\left(\frac{T}{10000}\right) + 1.62\left\{\log\left(\frac{T}{10000}\right)\right\}^2\right]$		11 12 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	$H^+ + e^- \rightarrow H + \gamma$	$k_{12,A} = 1.269 \times 10^{-13}\left(\frac{315614}{T}\right)^{1.503}$ $\times [1.0 + \left(\frac{604625}{T}\right)^{0.470}]^{-1.923}$ $k_{12,B} = 2.753 \times 10^{-14}\left(\frac{315614}{T}\right)^{1.500}$ $\times [1.0 + \left(\frac{115188}{T}\right)^{0.407}]^{-2.242}$	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

(Glover, Federrath, Mac Low, Klessen, in prep)

chemical model 2

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
		$= \exp[-2.0372609 \times 10^1$		
		$+ 1.13944933 \times 10^0 \ln T_e$		
		$- 1.4210135 \times 10^{-1} (\ln T_e)^2$		
		$+ 8.4644554 \times 10^{-3} (\ln T_e)^3$		
		$- 1.$[illegible]327641×10^{-3}[illegible]$\ln T_e)^4$		
		$+ 2.12$[illegible]$\times 10^{-4}$[illegible]$\ln T_e$[illegible]		
		$+$[illegible]0632[illegible]10^{-5}[illegible]$\ln T_e$[illegible]		
		$- 2.5850097 \times 10^{-5}$[illegible]$(\ln T_e)$[illegible]		
		$+ 2.4555012 \times 10^{-6} (\ln T_e)^8$		
		$- 8.0683825 \times 10^{-8} (\ln T_e)^9]$	$T_e > 0.1$ 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

(Glover, Federrath, Mac Low, Klessen, in prep)

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(Glover, Federrath, Mac Low, Klessen, in prep)

Table B1.

No.	Reaction	Rate coefficient	Notes	Ref.
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
		$= 1.02 \times 10^{-10} \exp\left(-\frac{914}{T}\right)$	$T > 2000$ K	36
39	$CH_2 + H \rightarrow CH + H_2$	$k_{39} =$ [illegible] $\times 10^{-11}$		37
40	$CH_2 + O \rightarrow CO + H + H$	$k_{40} =$ [illegible] $\times 10^{-10}$		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

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No.	Reaction	Rate coefficient	Ref.
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	$CH_2 + H^+ \rightarrow C^+ + He + H_2$	$k_{92} = 7.5 \times 10^{-10}$	28
93	$C_2 + He^+ \rightarrow C^+ + C + He$	$k_{93} =$ [illegible]	28
94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-9}$	28
95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10$[illegible]	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, in prep)

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No.	Reaction	Rate coefficient	Notes	Ref.
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	$CH_2 + He^+ \rightarrow C^+ + He + H_2$	$k_{92} = 7.5 \times 10^{-10}$		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
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
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

(Glover, Federrath, Mac Low, Klessen, in prep)

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No.	Reaction	Rate coefficient	Ref.
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
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	$C + \gamma \rightarrow C^+ + e^-$	$R_{171} = 3.1 \times 10^{-10}$	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, in prep)

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	$CH_2 + He^+ \rightarrow C^+ + He + H_2$	$k_{92} = 7.5 \times 10^{-10}$	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	$C + \gamma \rightarrow C^+ + e^-$			
172	$C^- + \gamma \rightarrow$			
173	$CH + \gamma \rightarrow$			
174	$CH + \gamma \rightarrow$			
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	$O^- + \gamma \rightarrow$			
183	$OH + \gamma \rightarrow$			
184	$OH + \gamma \rightarrow$			
185	$OH^+ + \gamma$			
186	$H_2O + \gamma$			
187	$H_2O + \gamma$			
188	$H_2O^+ + \gamma$			
189	$H_2O^+ + \gamma$			
190	$H_2O^+ + \gamma$			
191	$H_2O^+ + \gamma$			
192	$H_3O^+ + \gamma$			
193	$H_3O^+ + \gamma$			
194	$H_3O^+ + \gamma$			
195	$H_3O^+ + \gamma$			
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)

HI to H2 conversion rate

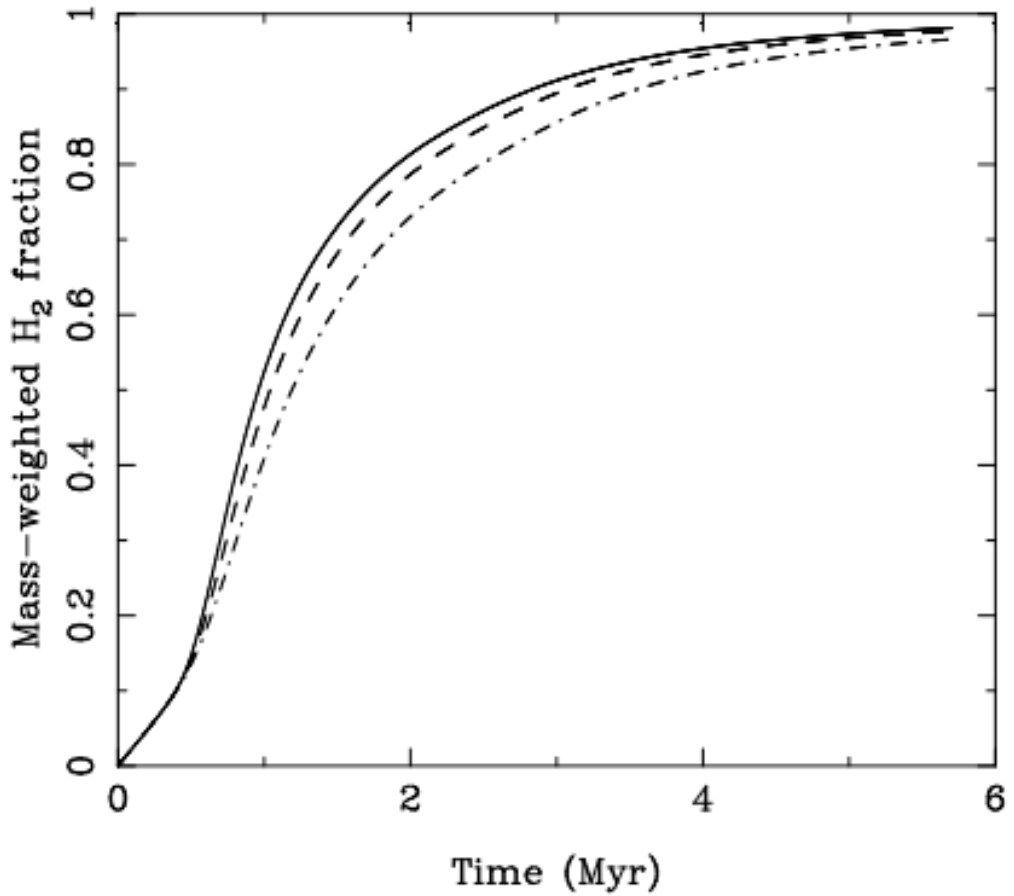


Figure 4. Time evolution of the mass-weighted H_2 abundance in simulations R1, R2 and R3, which have numerical resolutions of 64^3 zones (dot-dashed), 128^3 zones (dashed) and 256^3 zones (solid), respectively.

(Glover, Federrath, Mac Low, Klessen, in prep)

HI to H2 conversion rate

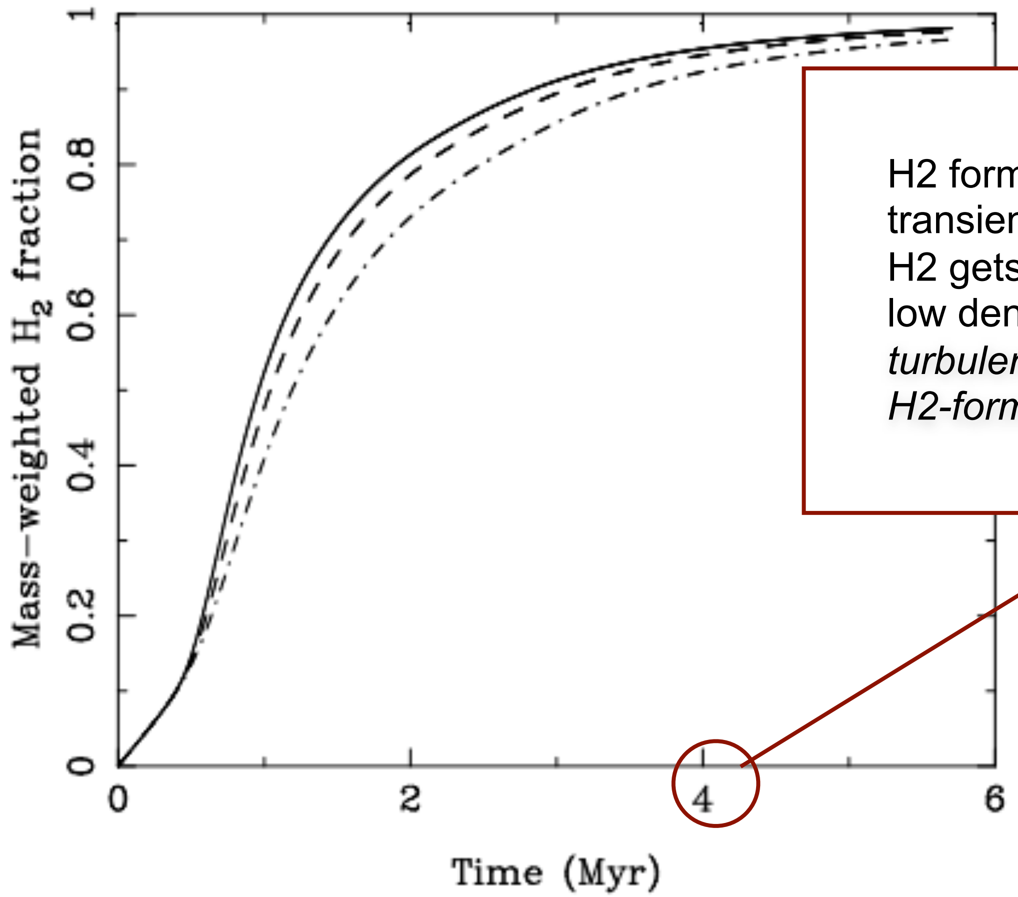


Figure 4. Time evolution of the mass-weighted H_2 abundance in simulations R1, R2 and R3, which have numerical resolutions of 64^3 zones (dot-dashed), 128^3 zones (dashed) and 256^3 zones (solid), respectively.

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

(Glover, Federrath, Mac Low, Klessen, in prep)

CO, C^+ formation rates

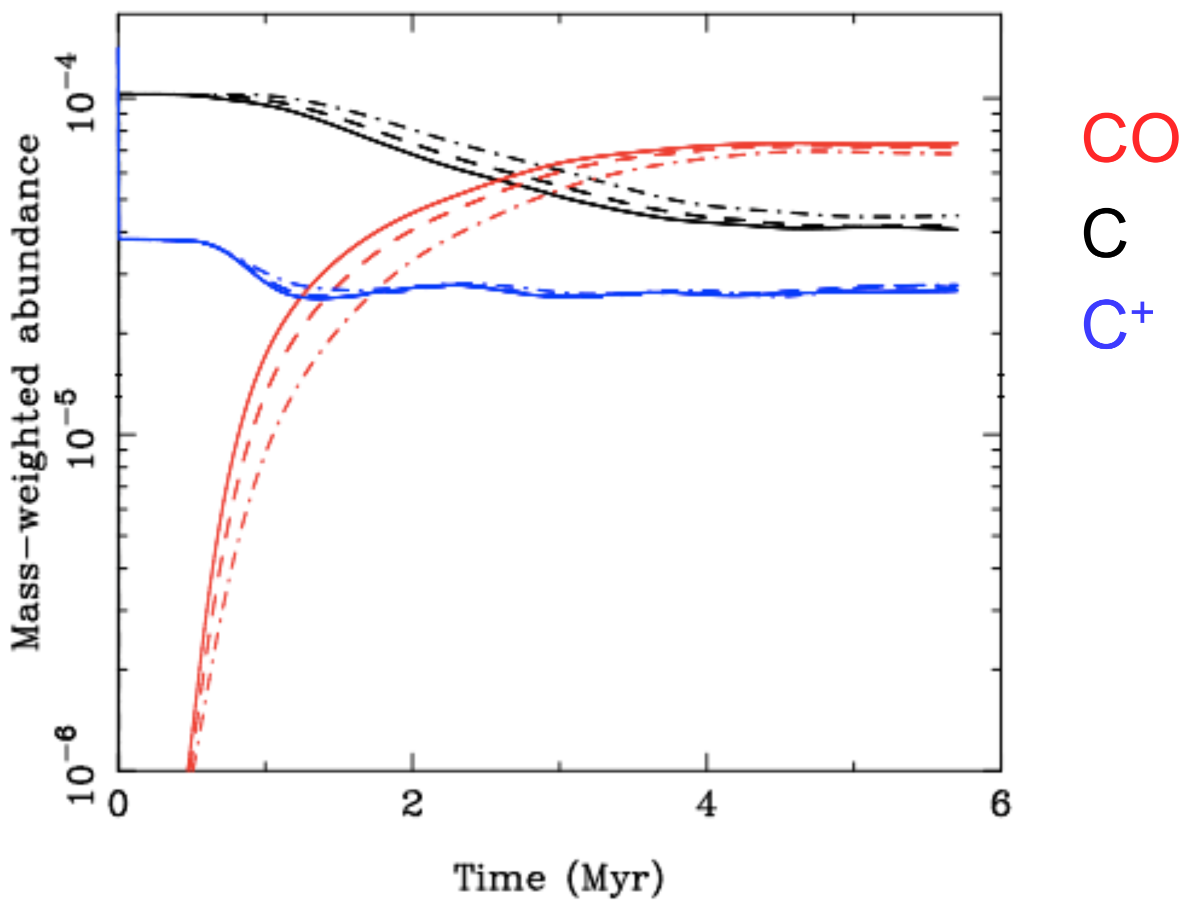
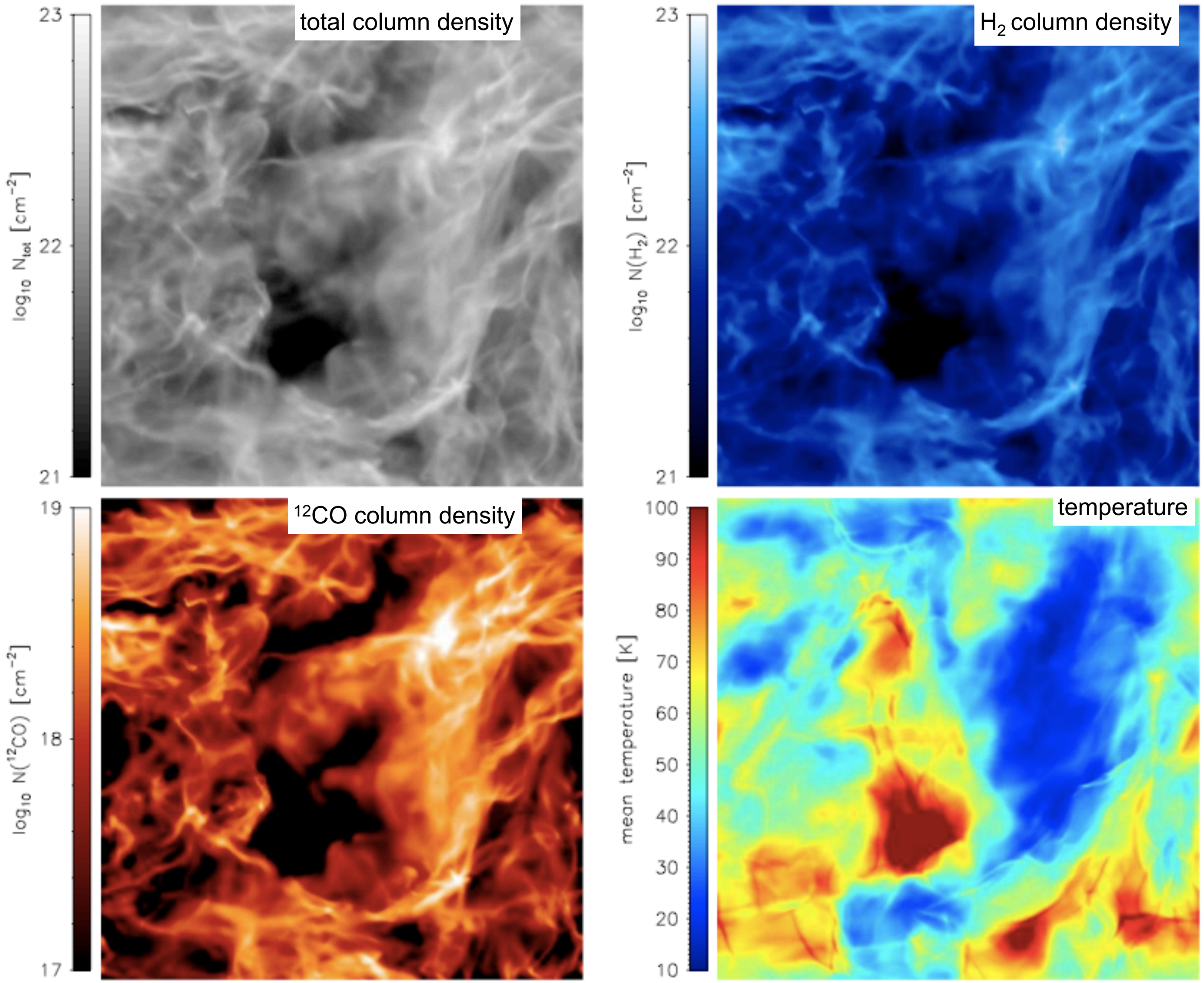


Figure 5. Time evolution of the mass-weighted abundances of atomic carbon (black lines), CO (red lines), and C^+ (blue lines) in simulations with numerical resolutions of 64^3 zones (dot-dashed), 128^3 zones (dashed) and 256^3 zones (solid).

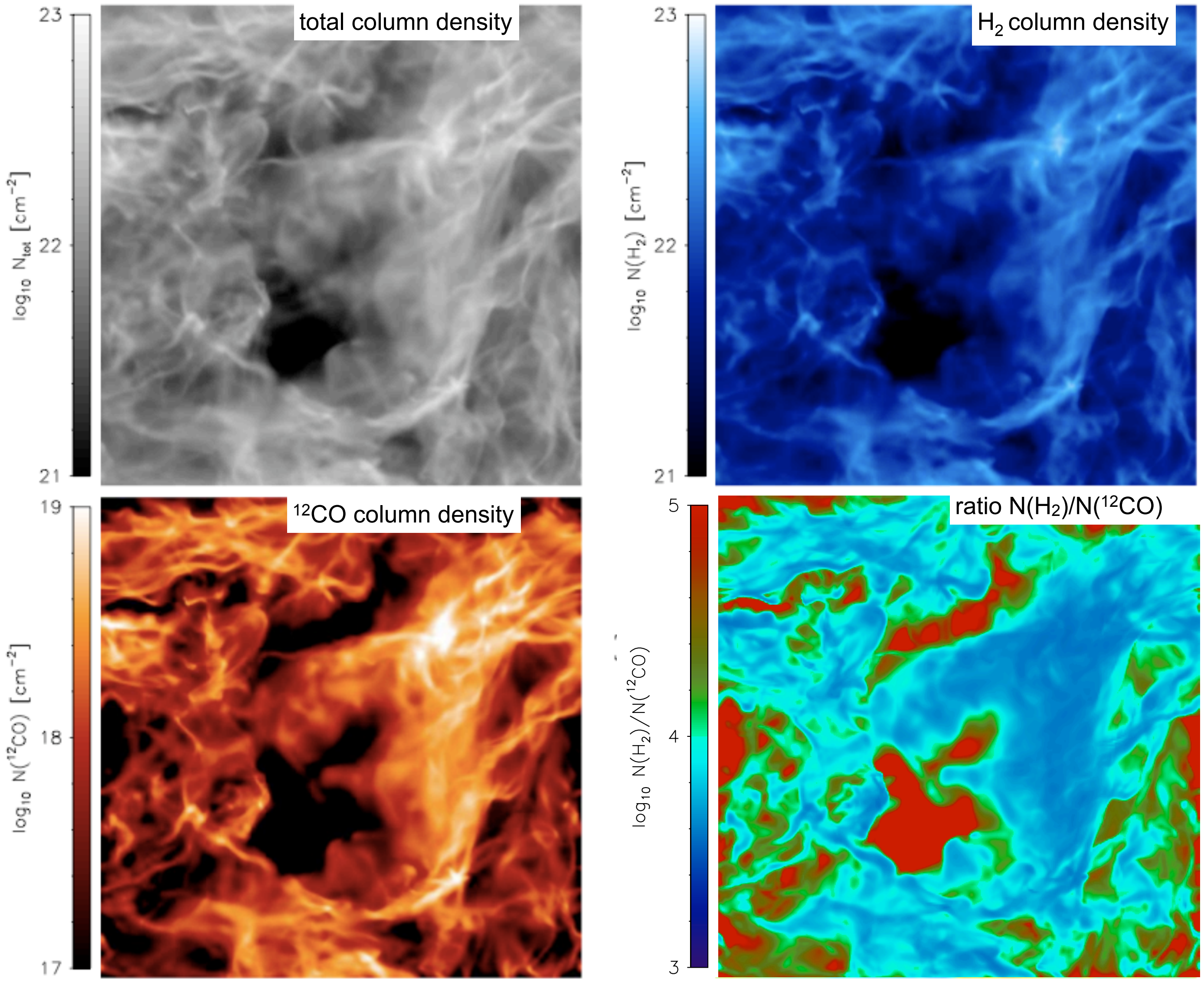
(Glover, Federrath, Mac Low, Klessen, in prep)

effects of chemistry 1



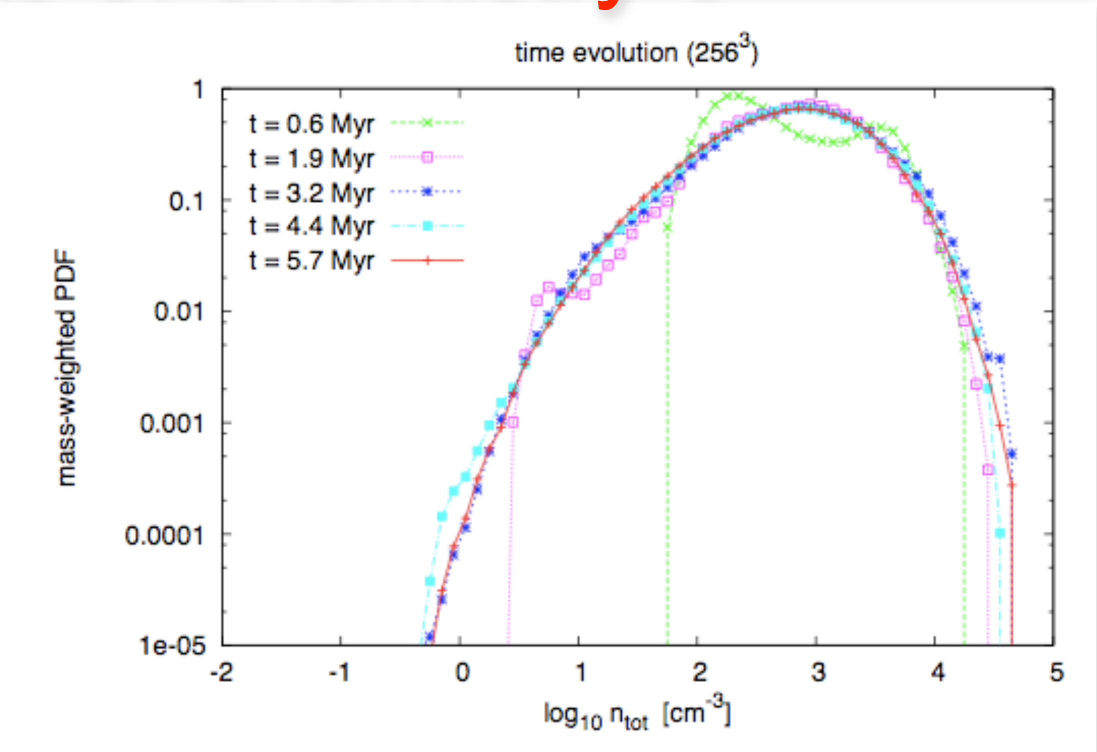
(Glover, Federrath, Mac Low, Klessen, in prep)

effects of chemistry 2



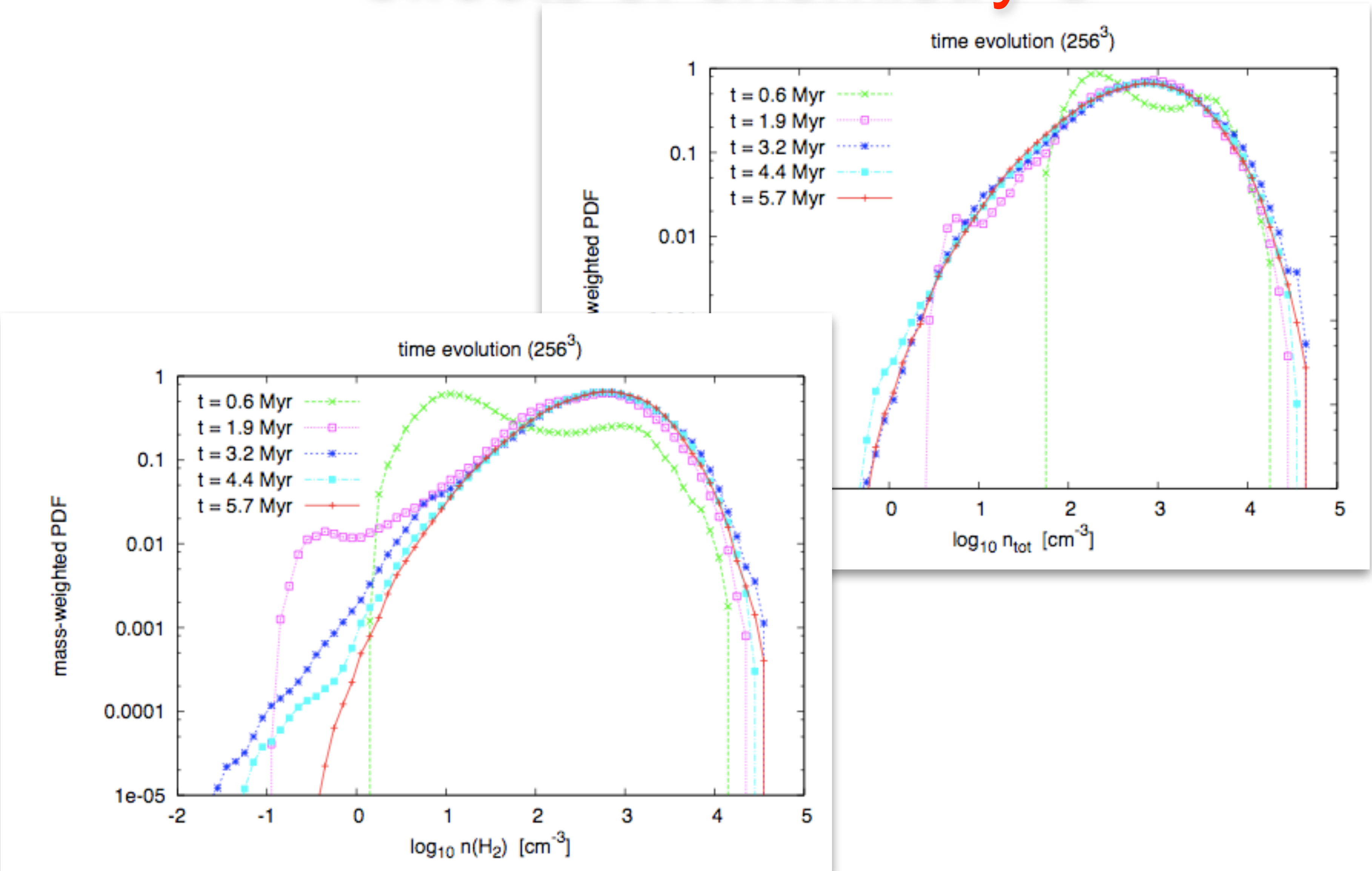
(Glover, Federrath, Mac Low, Klessen, in prep)

effects of chemistry 3



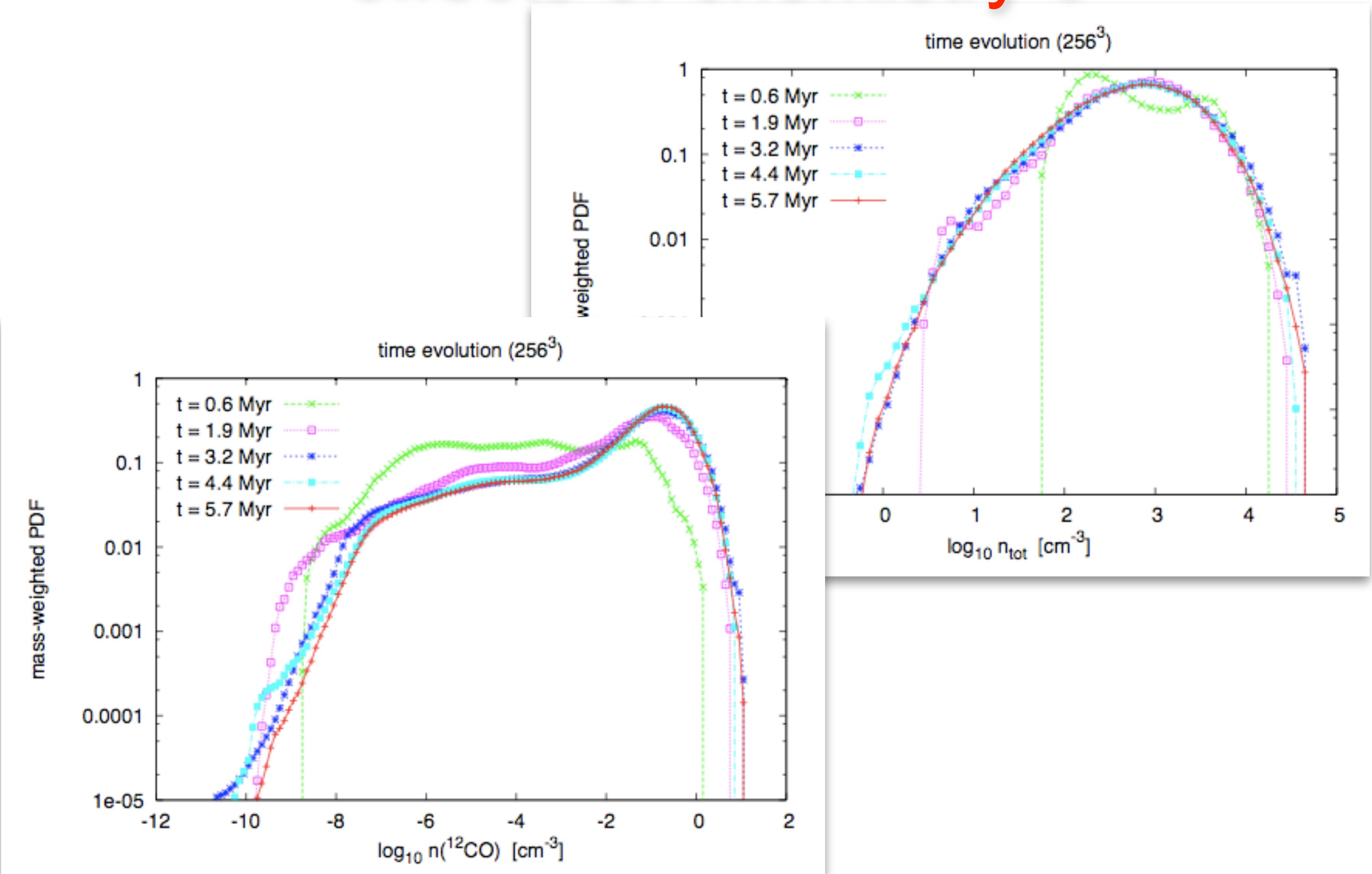
(Glover, Federrath, Mac Low, Klessen, in prep)

effects of chemistry 3



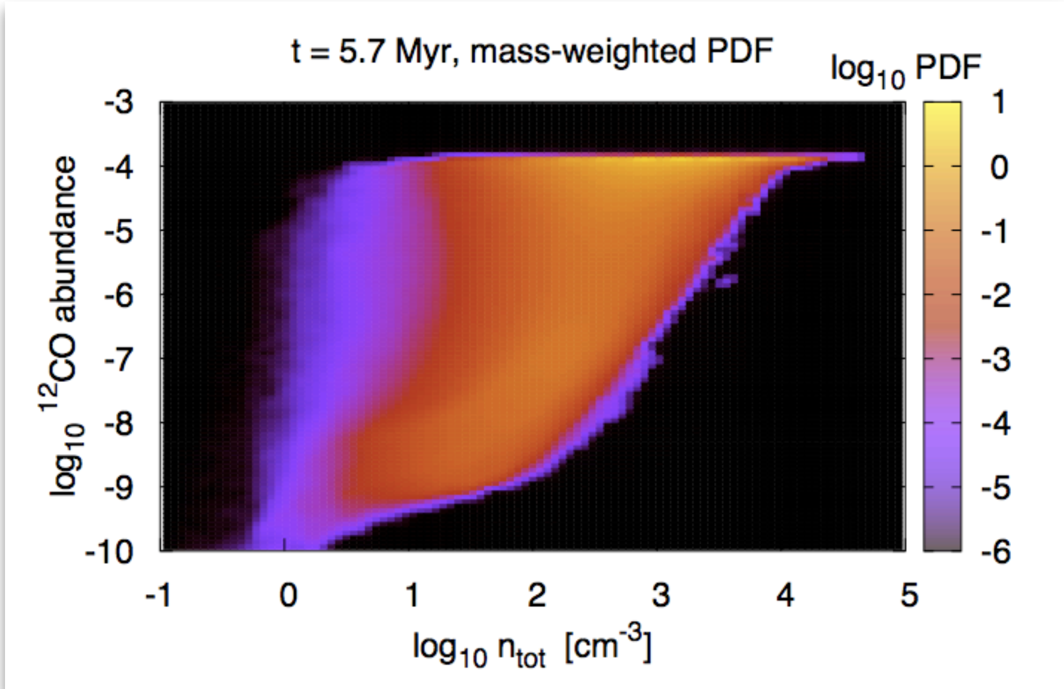
(Glover, Federrath, Mac Low, Klessen, in prep)

effects of chemistry 3



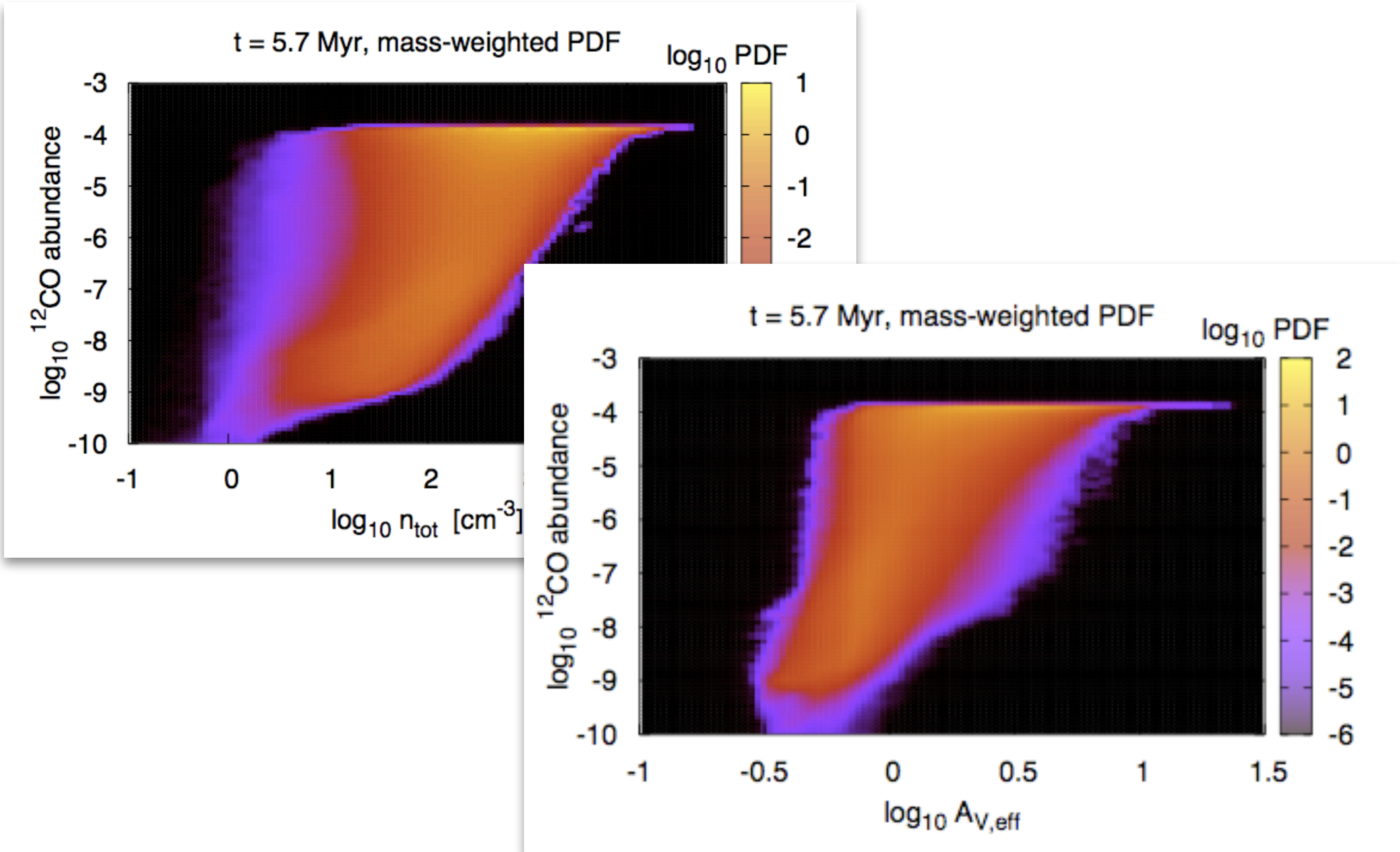
(Glover, Federrath, Mac Low, Klessen, in prep)

effects of chemistry 3



(Glover, Federrath, Mac Low, Klessen, in prep)

effects of chemistry 3



(Glover, Federrath, Mac Low, Klessen, in prep)

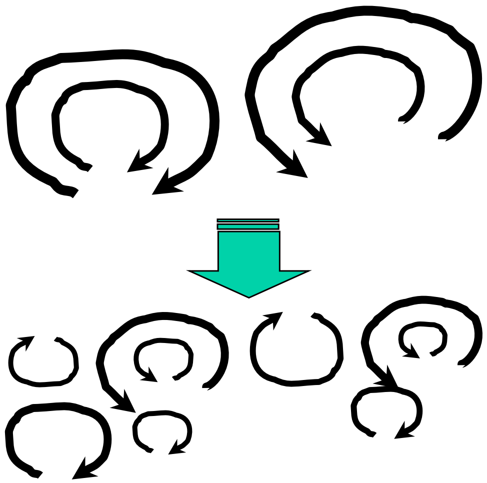
turbulence

Properties of turbulence

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

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

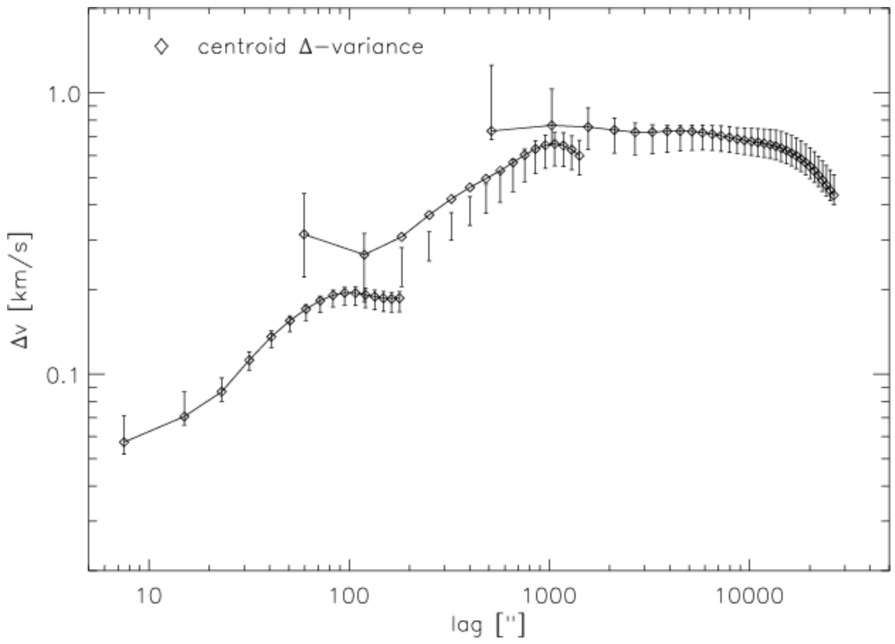
V= typical velocity on scale L, ν = viscosity, Re > 1000



- *vortex streching* --> 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)

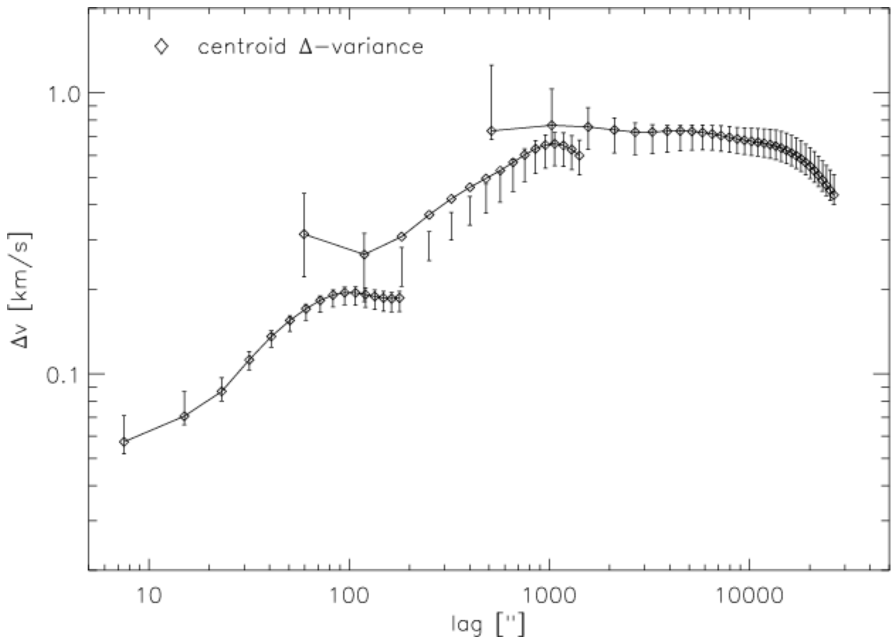
what drives turbulence?



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?

what drives turbulence?

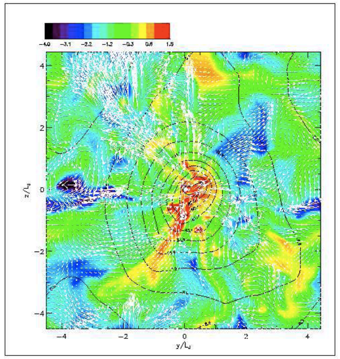


Polaris flare (from Ossenkopf & Mac Low 2002)

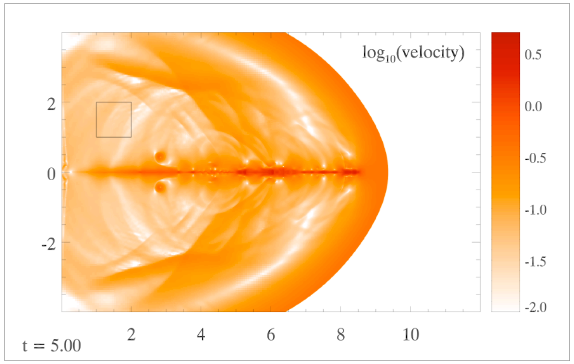
- turbulence characteristics
  - molecular cloud turbulence seems to be dominated by large-scale models
  - consistent with external driving
  - *convergent flows?*
    → the same process that creates the cloud supplies internal turbulence ..
    → caused by
      - *gravity (spiral shocks),* supernovae,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

what drives turbulence?

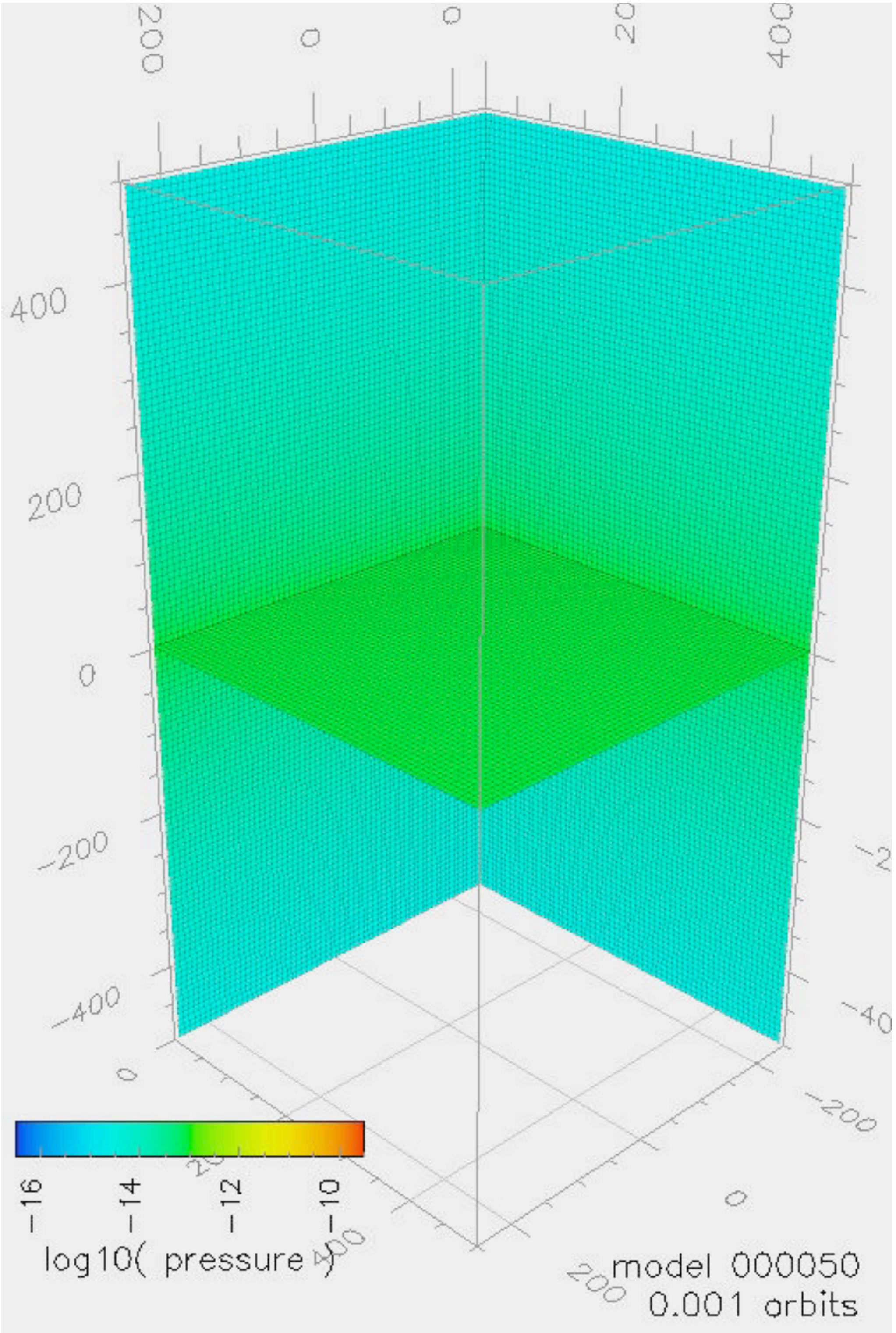
- molecular cloud turbulence is be dominated by *large-scale modes*
  - *"external"* sources such as supernovae, expanding HII regions, or large-scale gravitational process (spiral waves, accretion, etc)
- some words on *"internal"* sources
  - jets / outflow can only work after onset of star formation
    → what about turbulence in non-star forming parts of clouds, or during initial phases?
  - debate on effectiveness of internal sources for driving supersonic turbulence
    (Li & Nakamura + Wang et al. vs. Banerjee, Klessen, Fendt)



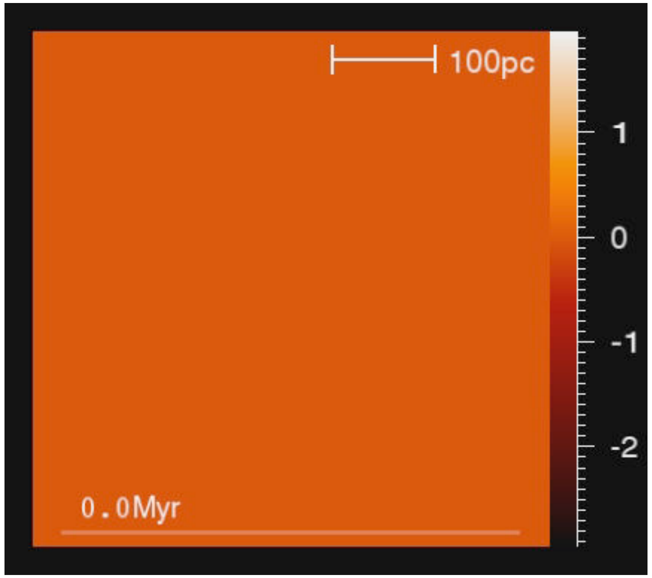
(Nakamura & Li 2007)



(Banerjee, Klessen, Fendt 2008)



from PhD thesis of Oliver Gressel (AIP)

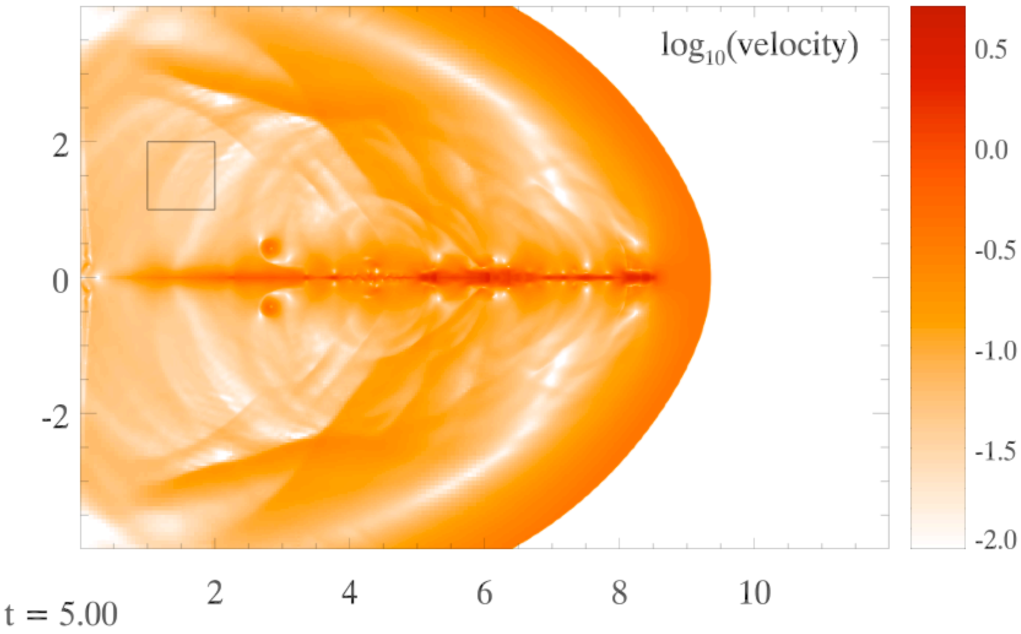


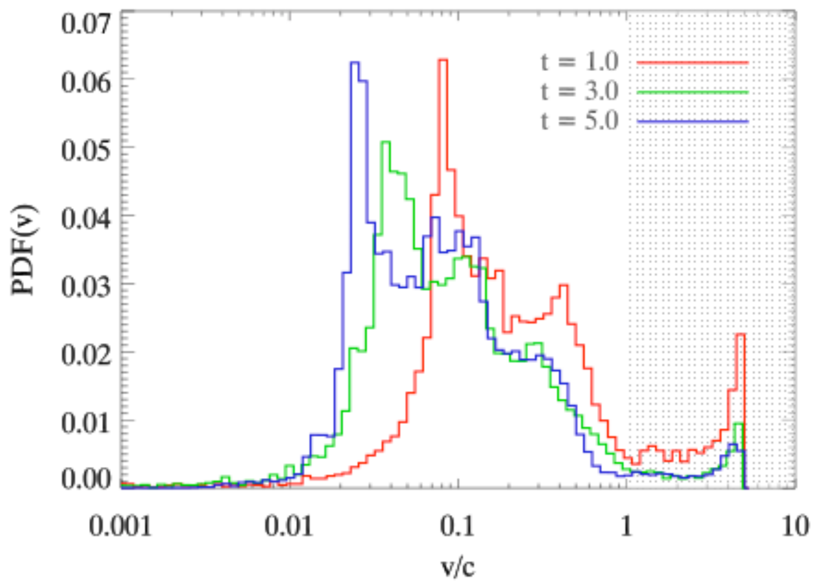
from PhD thesis of Oliver Gressel (AIP)

also work by
deAvillez & Breitschwerdt
Oishi & Mac Low
Kim & Ostriker
Shetty & Ostriker
and many others...

local feedback

- individual jets cannot drive supersonic turbulence in a space-filling way → need additional physics

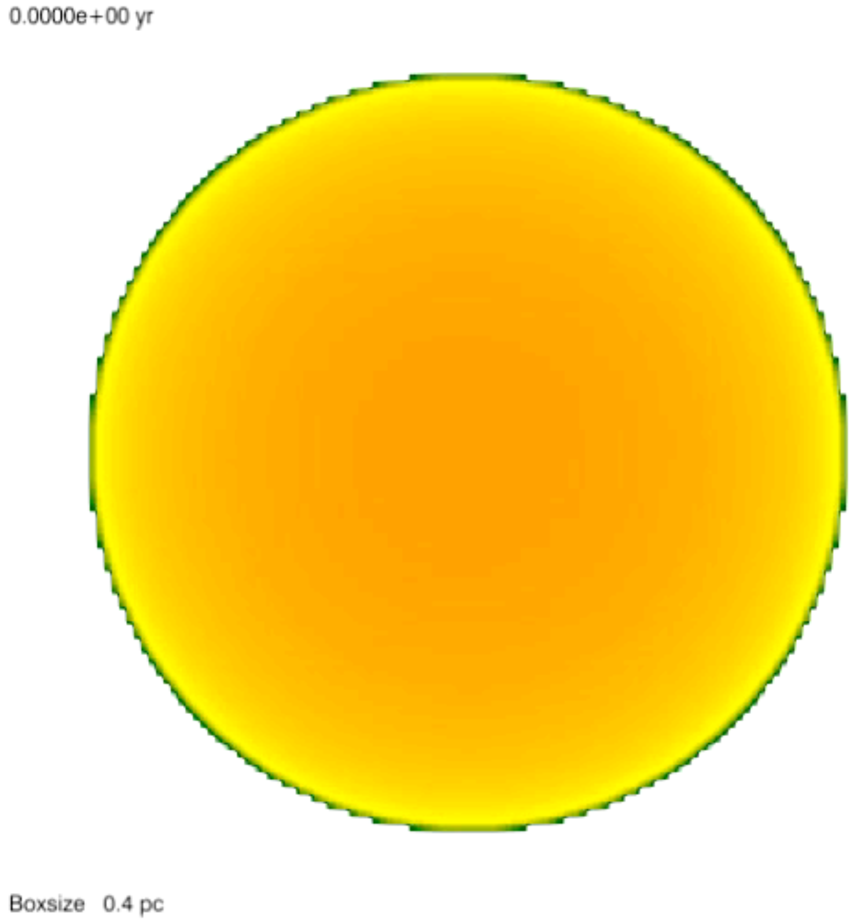




Banerjee, Klessen, & Fendt (2008)

cluster forming cloud with jets

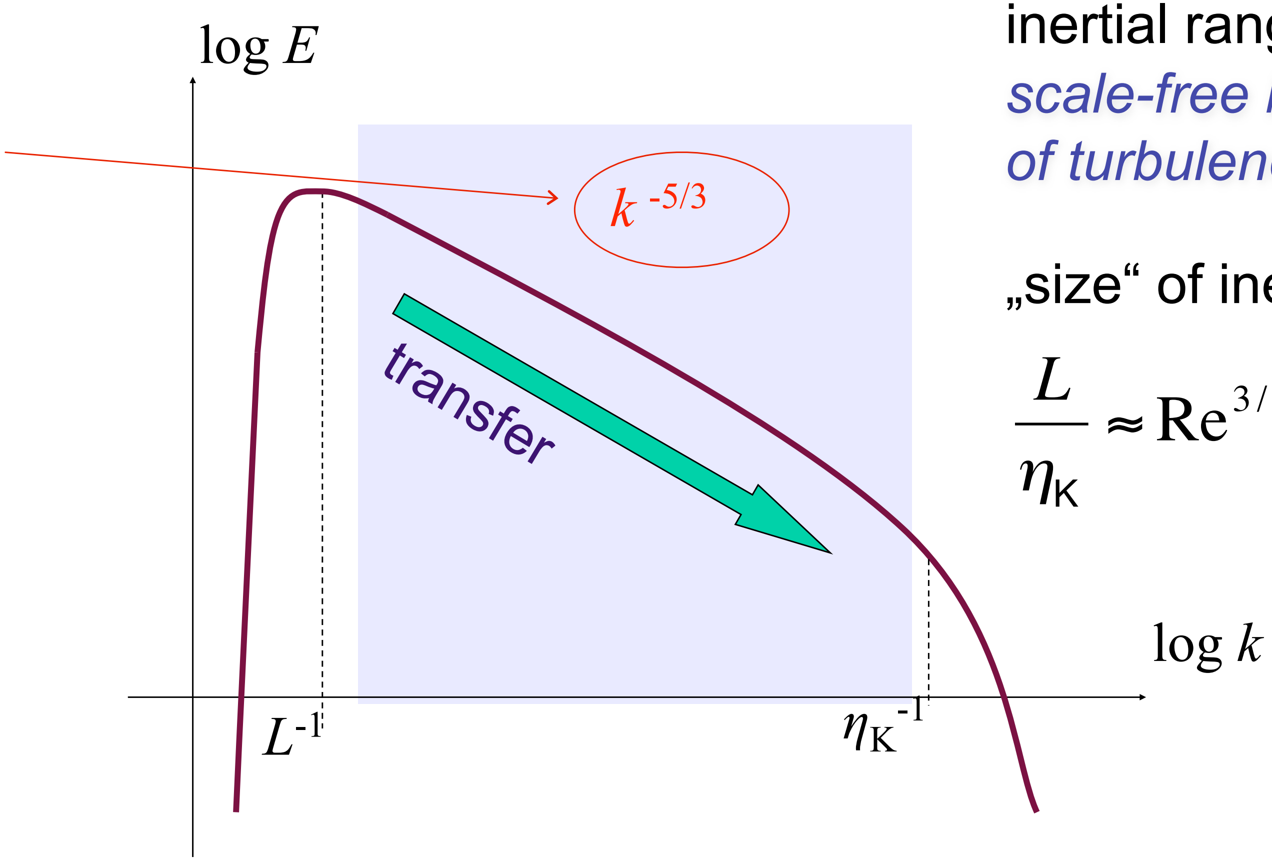
- jets from cluster with self-gravity with AMR code FLASH



Banerjee et al. (very preliminary study)

Turbulent cascade

Kolmogorov (1941) theory
incompressible turbulence



energy
input
scale

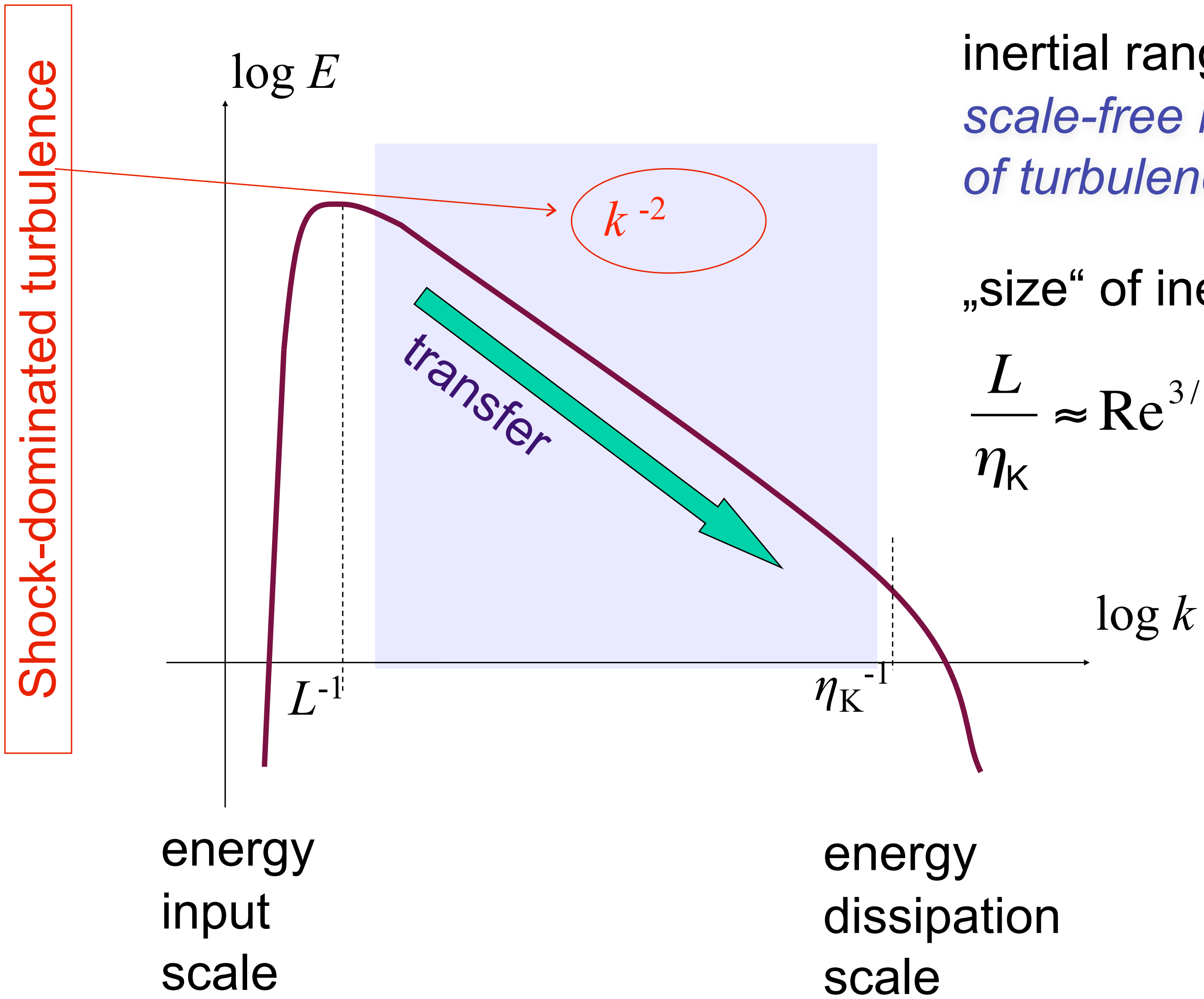
energy
dissipation
scale

inertial range:
scale-free behavior of turbulence

„size“ of inertial range:

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

Turbulent cascade

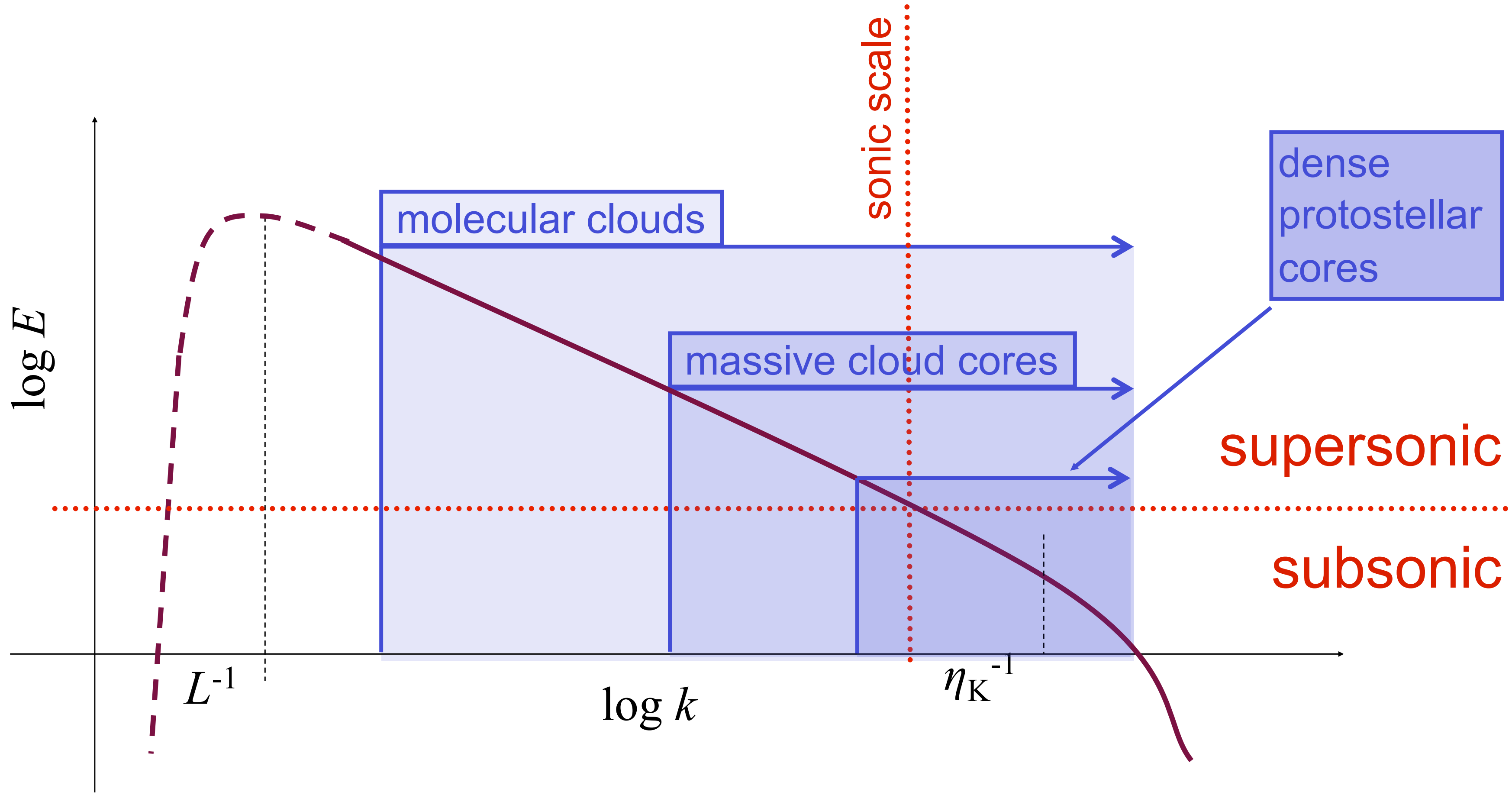


inertial range:
scale-free behavior of turbulence

„size“ of inertial range:

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

Turbulent cascade in ISM



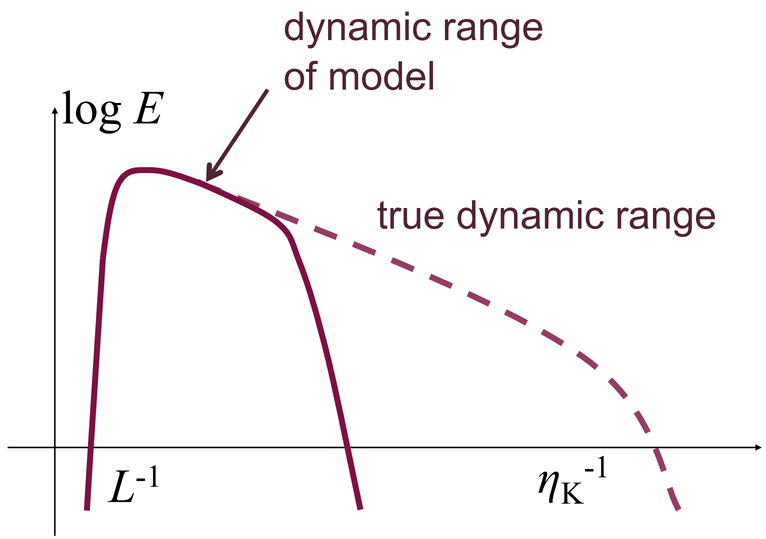
energy source & scale
NOT known
(supernovae, winds,
spiral density waves?)

σ_{rms} << 1 km/s
$M_{rms} \leq 1$
L ≈ 0.1 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/ν ***(Re_{nature} >> 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?



compressive vs. rotational driving

- statistical characteristics of turbulence depend strongly on „type“ of driving
- example: dilatational vs. solenoidal driving
- question: what drives ISM turbulence on different scales?

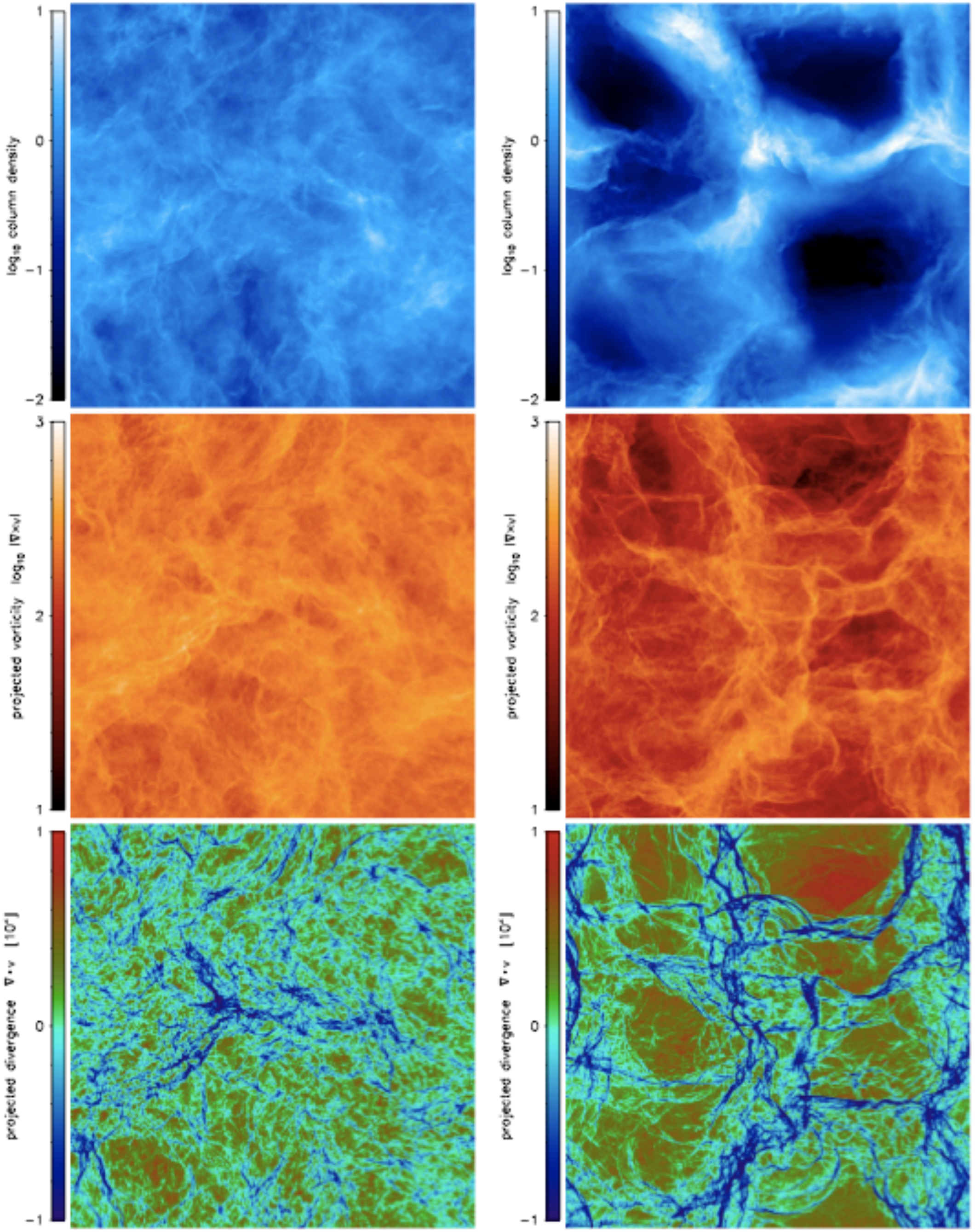
dilatational vs. solenoidal

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 $|\nabla \times v|$. 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 $\nabla \cdot v$ showing the positions of shocks. Negative divergence corresponds to compression, while positive divergence corresponds to rarefaction.

dilatational vs. solenoidal

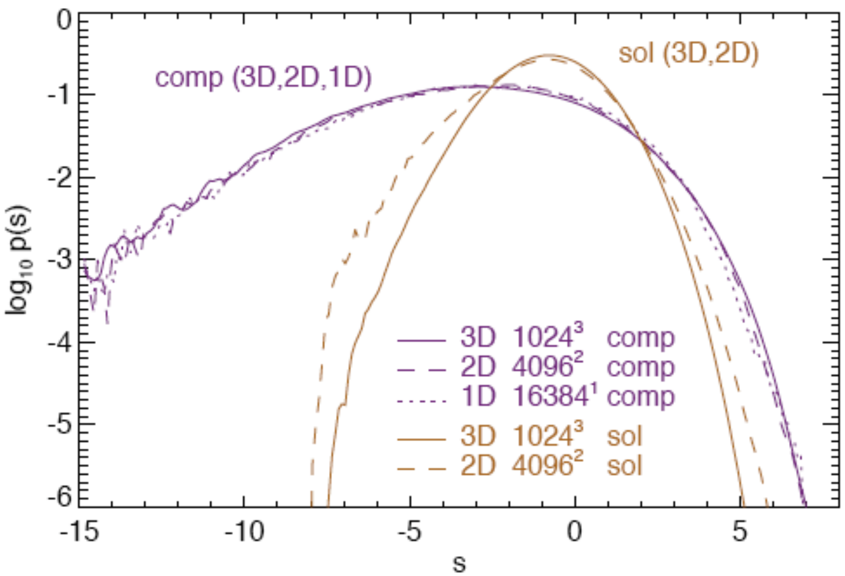


FIG. 3.— Volume-weighted density PDFs $p(s)$ obtained from 3D, 2D and 1D simulations with compressive forcing and from 3D and 2D simulations using solenoidal forcing. Note that in 1D, only compressive forcing is possible as in the study by Passot & Vázquez-Semadeni (1998). As suggested by eq. (5), compressive forcing yields almost identical density PDFs in 1D, 2D and 3D with $b\sim1$, whereas solenoidal forcing leads to a density PDF with $b\sim1/2$ in 2D and with $b\sim1/3$ in 3D.

- 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

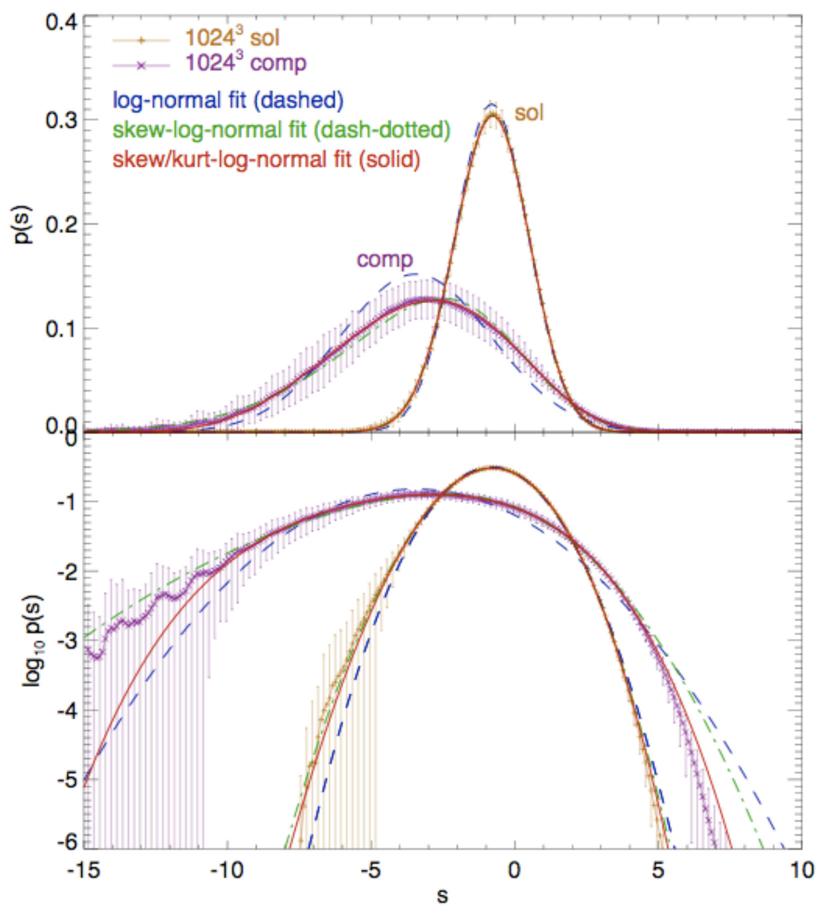
$$b = 1 + \left[\frac{1}{D} - 1\right]\zeta = \begin{cases} 1 - \frac{2}{3}\zeta & \text{, for } D = 3 \\ 1 - \frac{1}{2}\zeta & \text{, for } D = 2 \\ 1 & \text{, for } D = 1 \end{cases}$$

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

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

Federrath, Klessen, Schmidt (2008a)

dilatational vs. solenoidal



good fit needs 3rd and 4th moment of distribution!

Federrath, Klessen, Schmidt (2008b)

- density pdf depends on "dimensionality" of driving
  → is that a problem for the Krumholz & McKee model of the SF efficiency?
- density pdf of compressive driving is *NOT log-normal*
  → is that a problem for the Padoan & Nordlund IMF model?
- most "physical" sources should be *compressive* (convergent flows from spiral shocks or SN)

effects of chemistry 4

- 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!
    <-- gravity (poster by Kim), driving scheme (Federrath et al. 2008), EOS (Hennebelle & Audit 2009)

density pdf

1200^3 hydrodynamic simulation

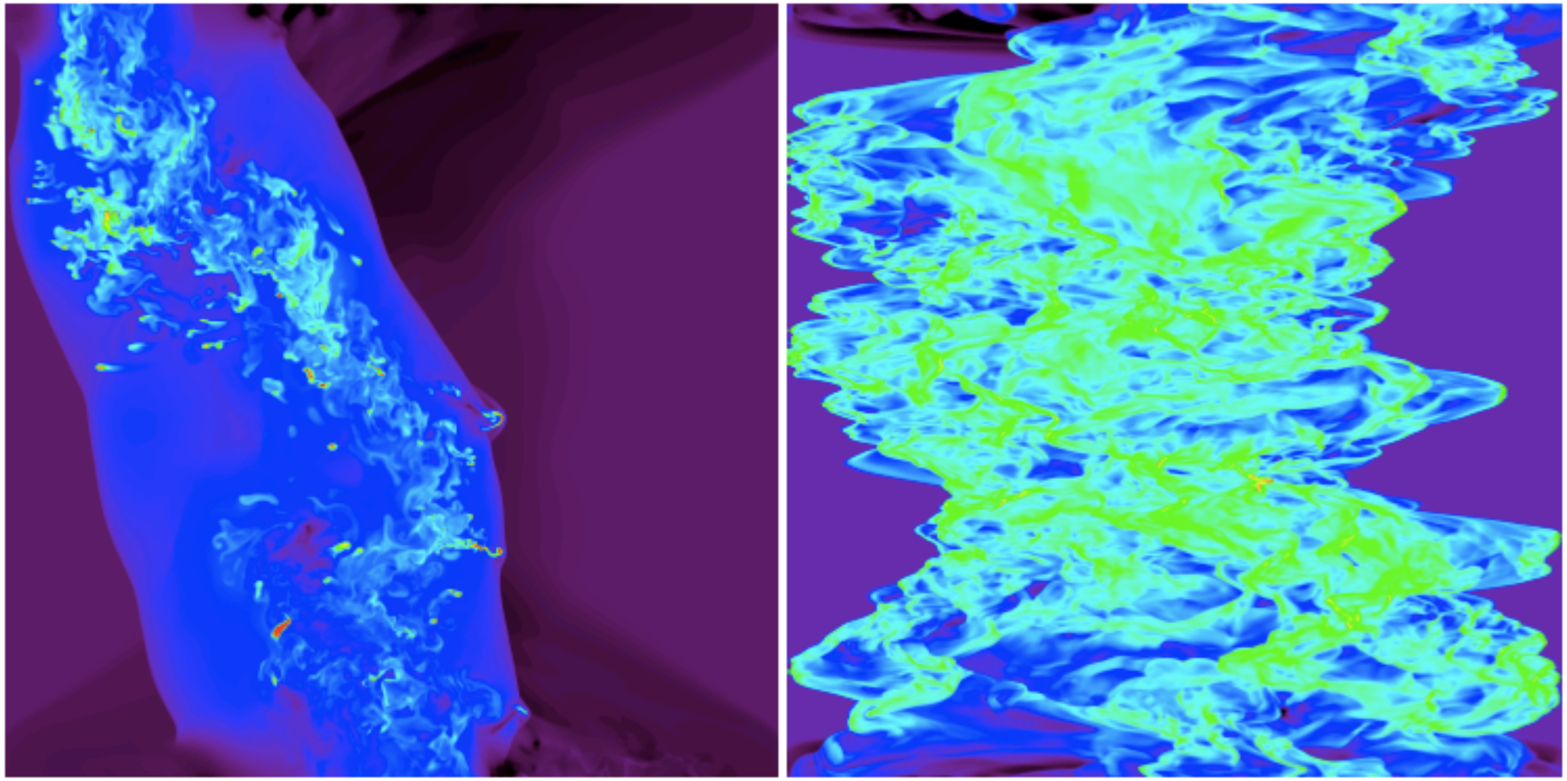


Fig. 3. Density cut through the simulations. The left plot corresponds to the 2-phase run and the right one to the isothermal run. Dark-blue, blue, green and red correspond respectively to densities of the order of 1 cm^{-3}, 3 cm^{-3}, 20 cm^{-3} and 100 cm^{-3}.

(Audit & Hennebelle, submitted)

density pdf

1200^3 hydrodynamic simulation

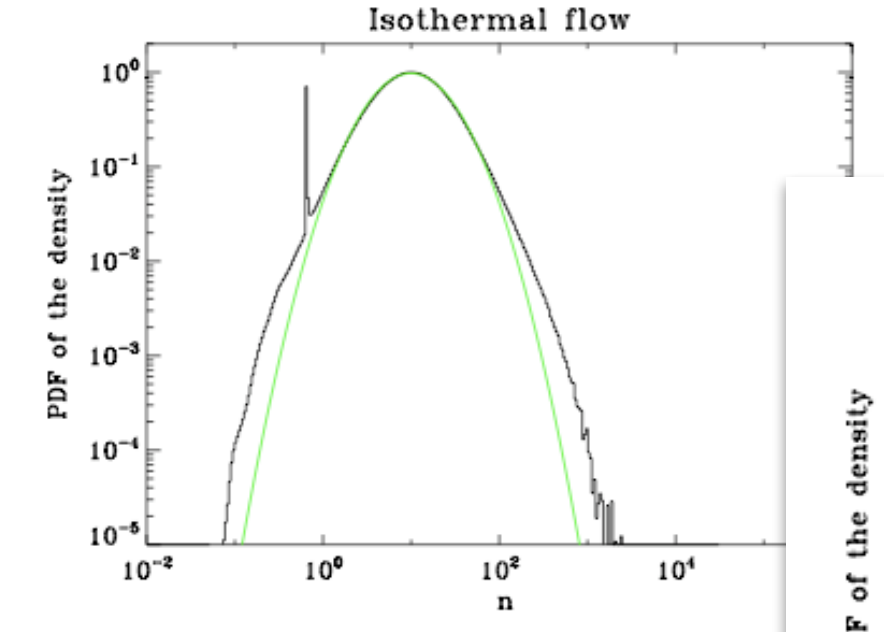


Fig. 5. Probability distribution function of the density f
isothermal run.

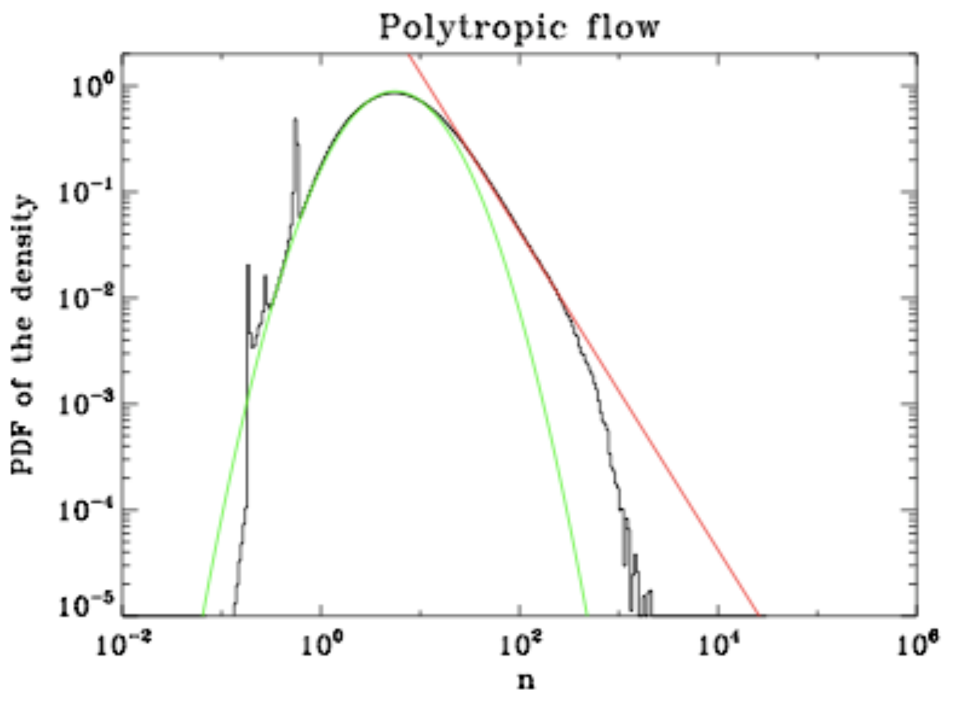


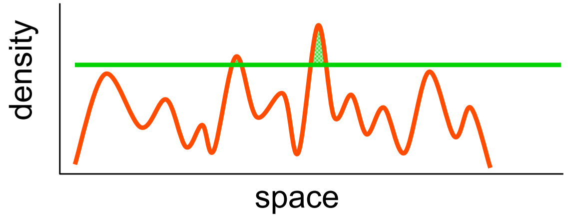
Fig. 6. Probability distribution function of the density for the polytropic run.

(Audit & Hennebelle, submitted)

basic idea

dynamical SF in a nutshell

- interstellar gas is highly *inhomogeneous*
  - *gravitational instability*
  - *thermal instability*
  - *turbulent compression* (in shocks $\delta\rho/\rho \propto \mathcal{M}^2$; in atomic gas: $\mathcal{M} \approx 1...3$)



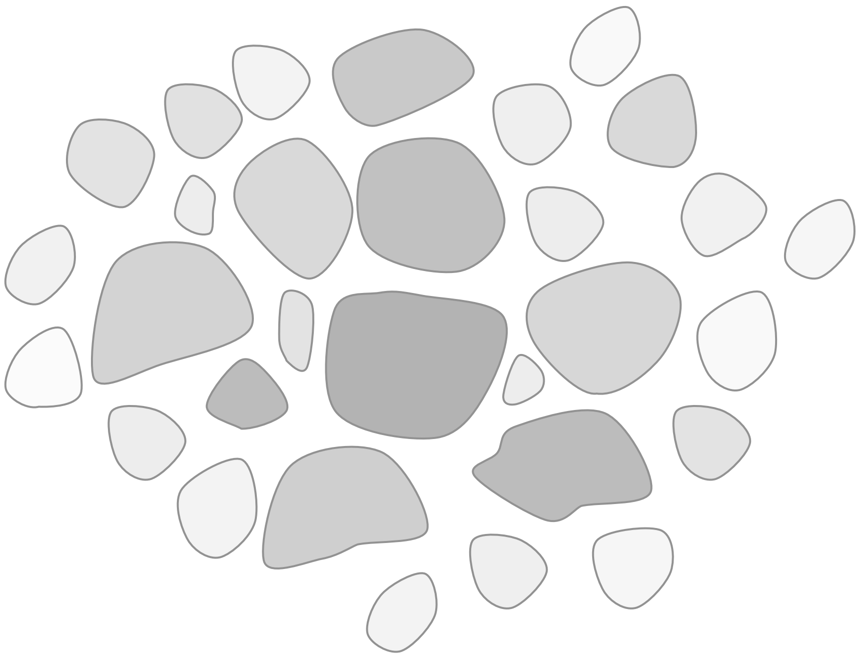
- cold *molecular clouds* can form rapidly in high-density regions at *stagnation points* of *convergent large-scale flows*
  - chemical *phase transition*: atomic → molecular
  - process is *modulated* by large-scale *dynamics* in the galaxy
- inside *cold clouds:* turbulence is highly supersonic ($\mathcal{M} \approx 1...20$)
  → *turbulence* creates large density contrast,
  gravity selects for collapse

  ⟶ ***GRAVOTUBULENT FRAGMENTATION***
- *turbulent cascade:* local compression *within* a cloud provokes collapse → formation of individual *stars* and *star clusters*

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

Formation and evolution of cores

What happens to distribution of cloud cores?



Two exteme cases:

(1) turbulence dominates energy budget:

$\alpha = E_{kin}/|E_{pot}| > 1$

--> individual cores do *not* interact

--> *collapse* of *individual* cores dominates *stellar mass growth*

--> *loose cluster of low-mass stars*

(2) turbulence decays, i.e. gravity dominates:

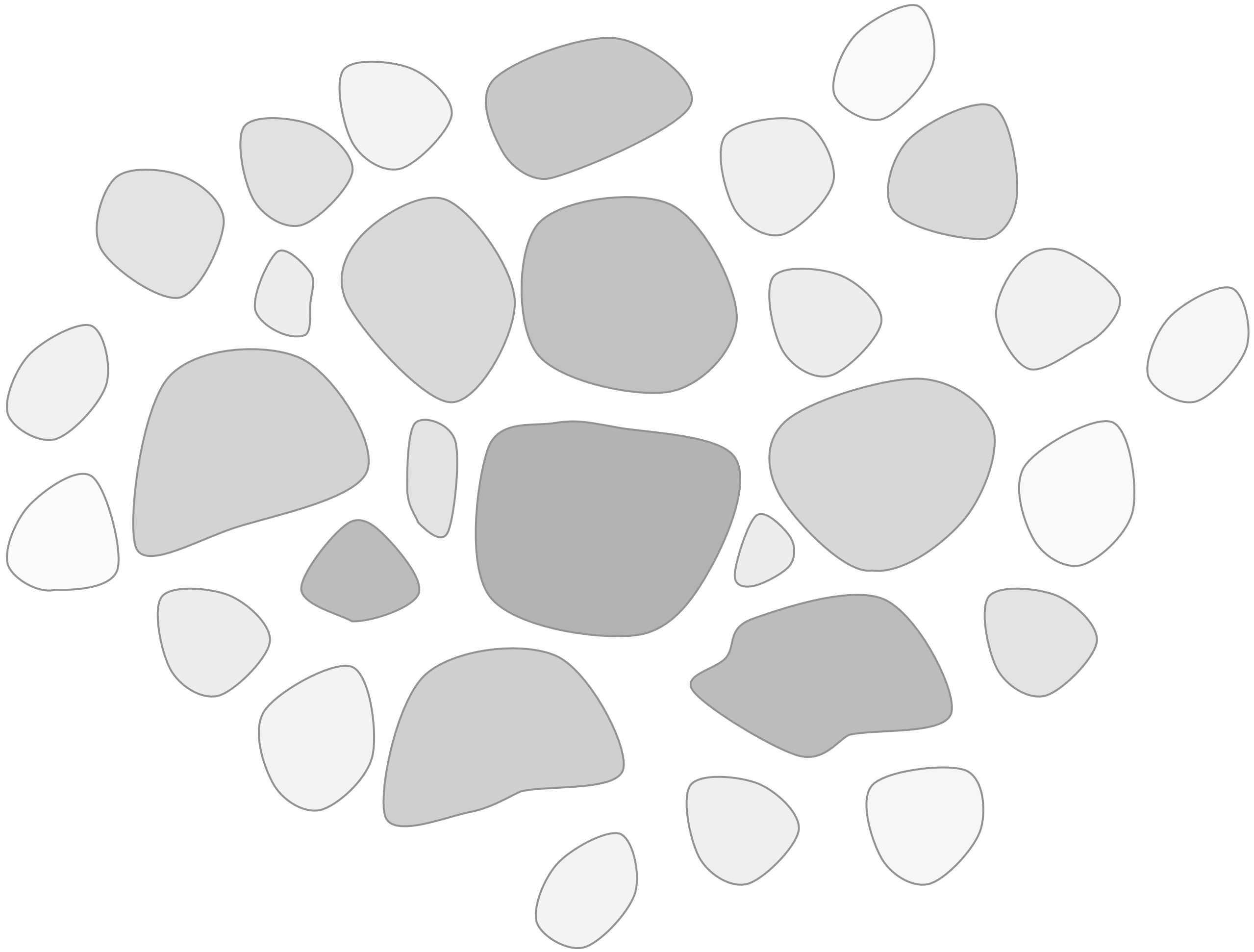
$\alpha = E_{kin}/|E_{pot}| < 1$

--> *global contraction*

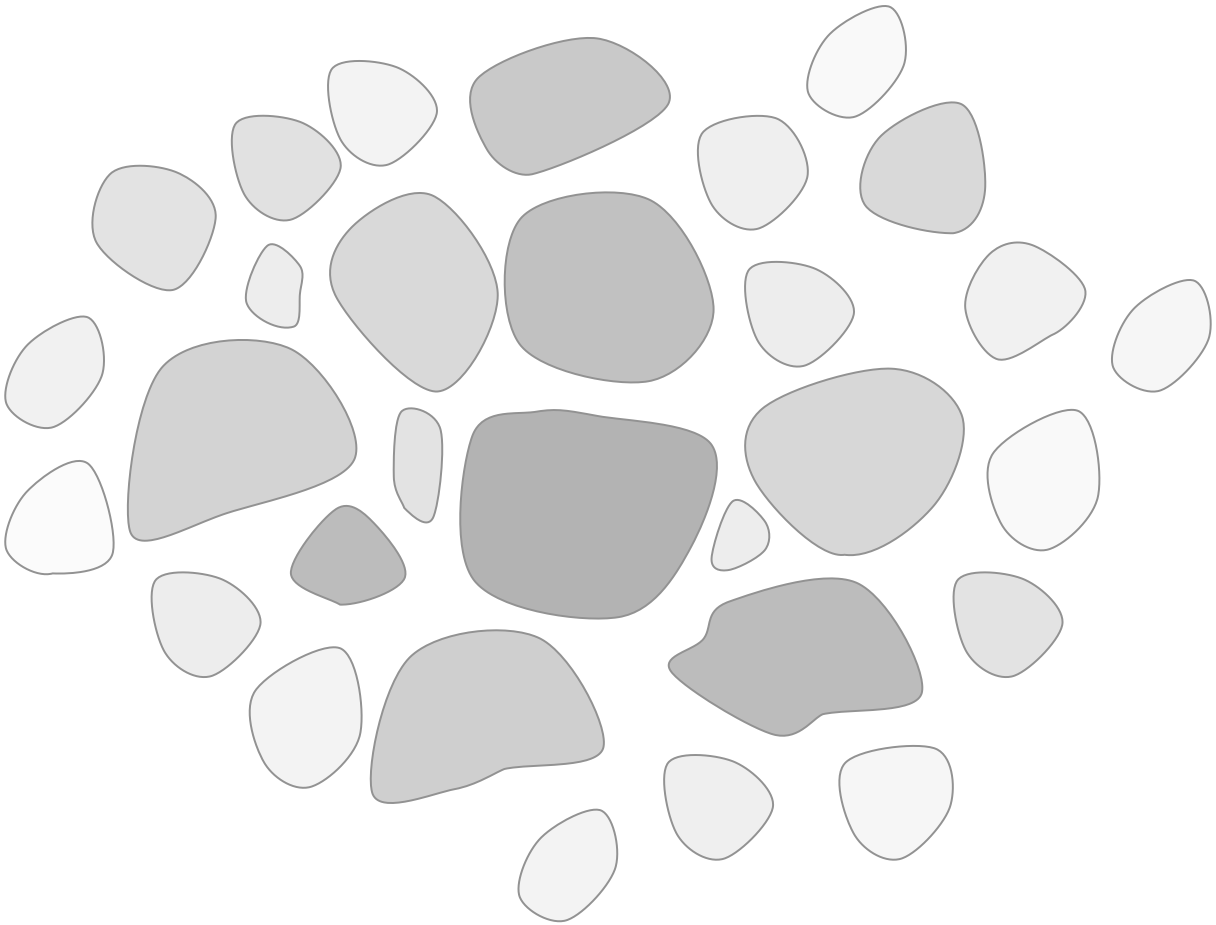
--> core do *interact* while collapsing

--> *competition* influences *mass growth*

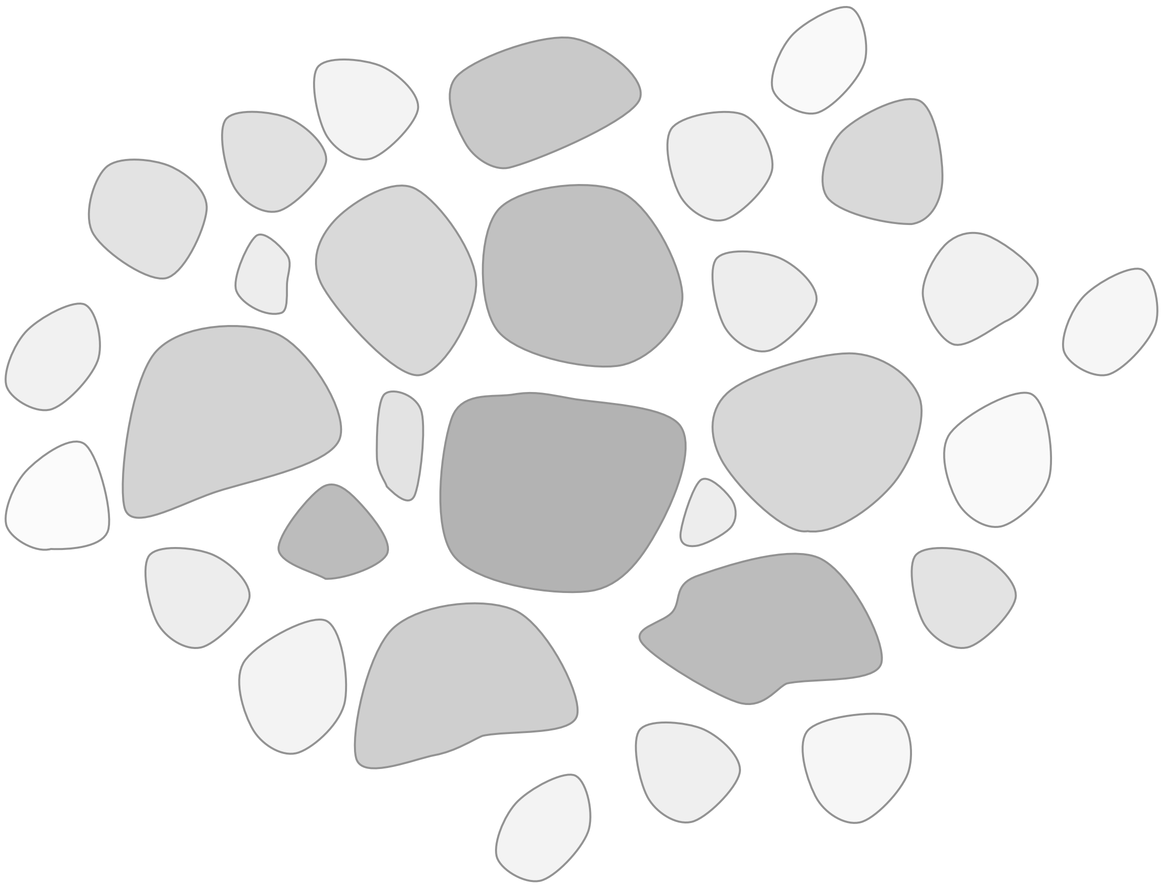
--> *dense cluster with high-mass stars*



turbulence creates a hierarchy of clumps



as turbulence decays locally, contraction sets in



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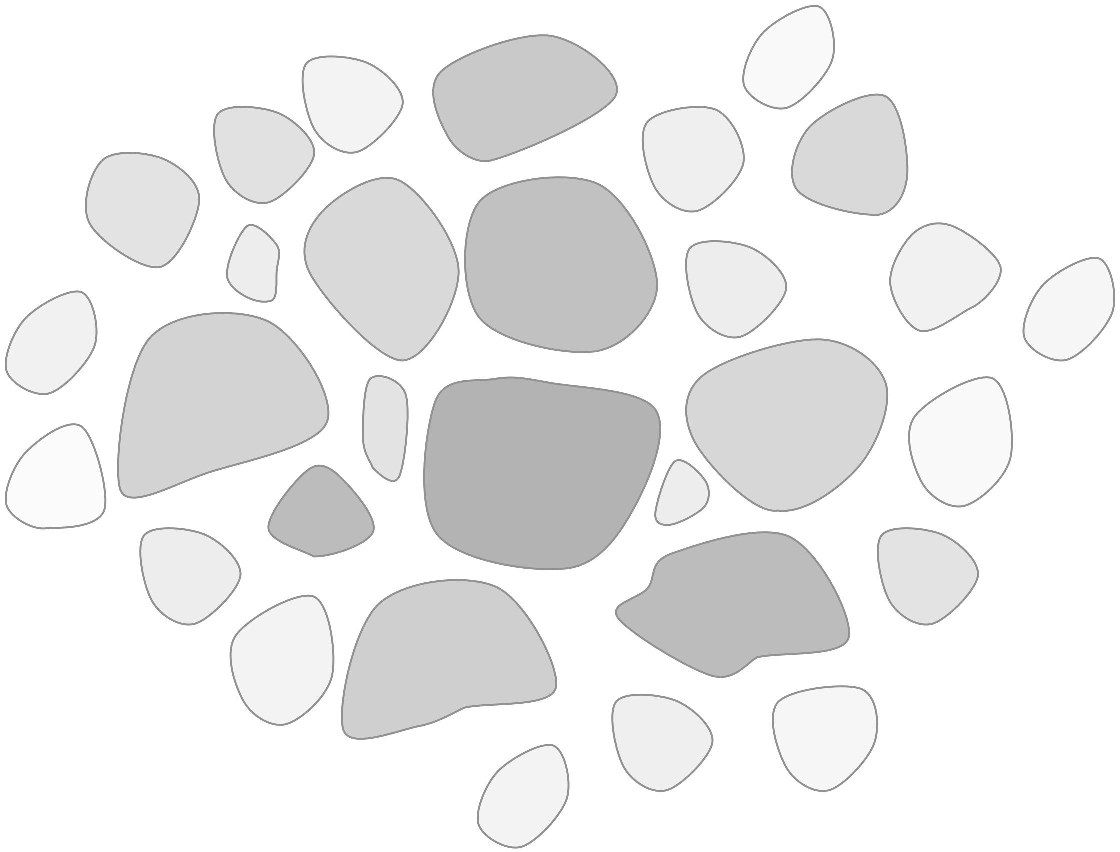
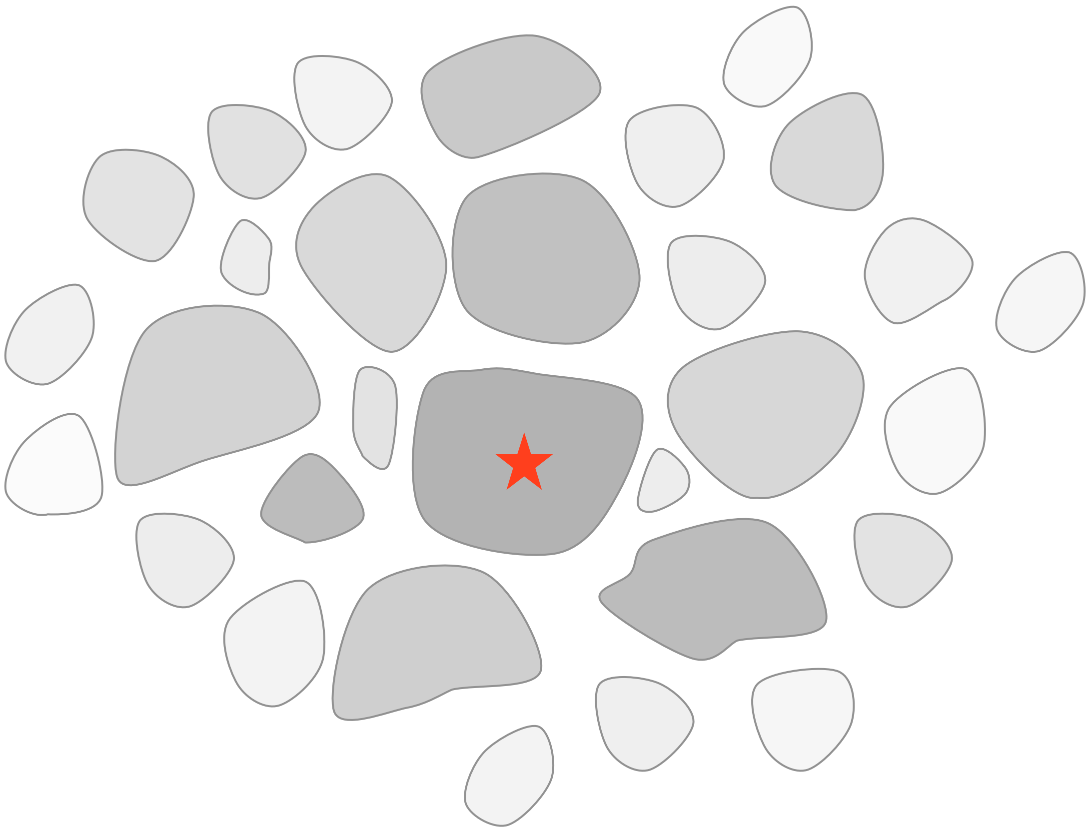


while region contracts, individual clumps collapse to form stars



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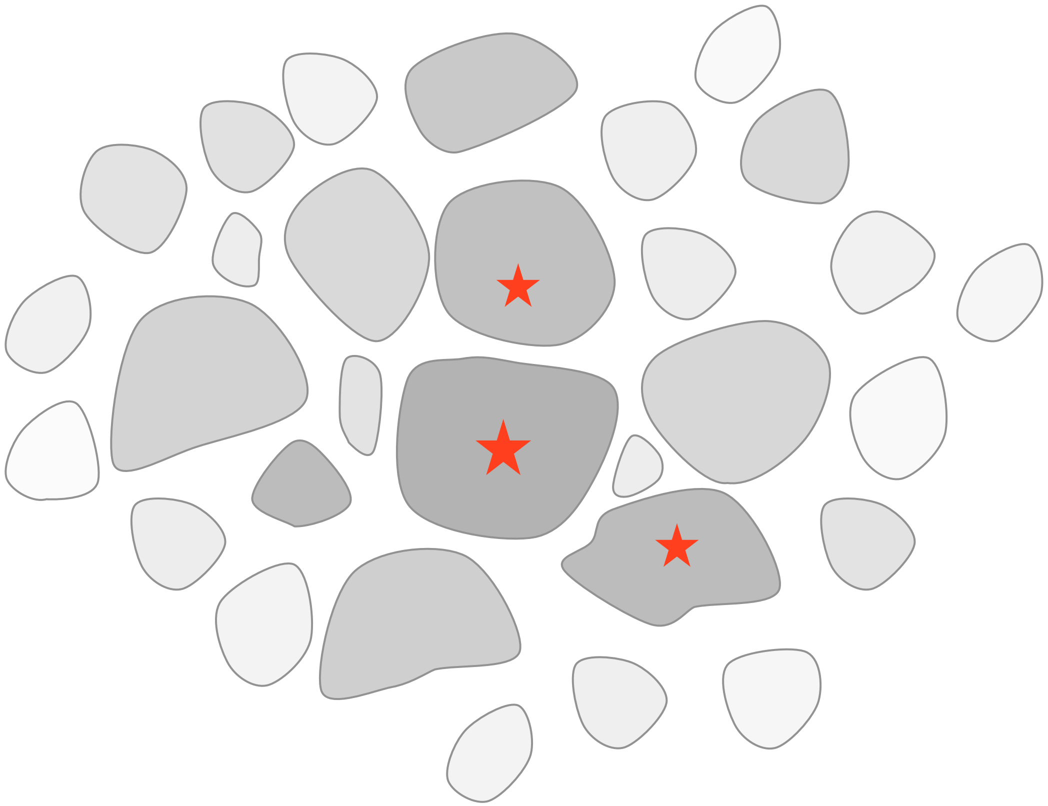
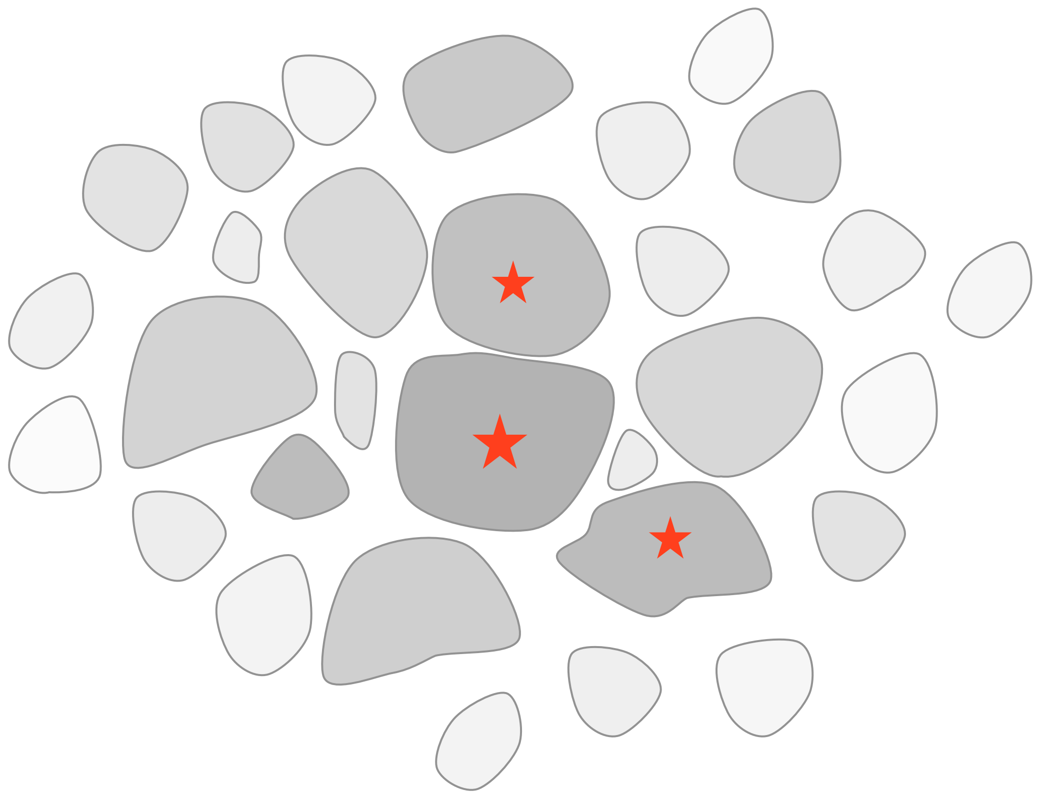


individual clumps collapse to form stars



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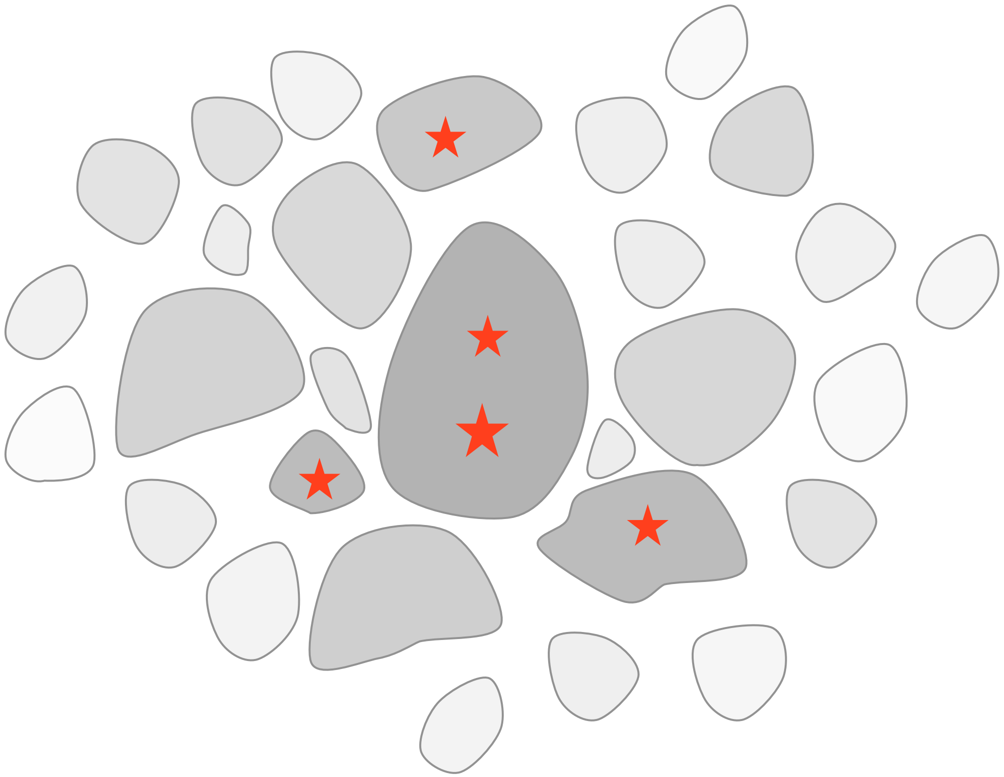
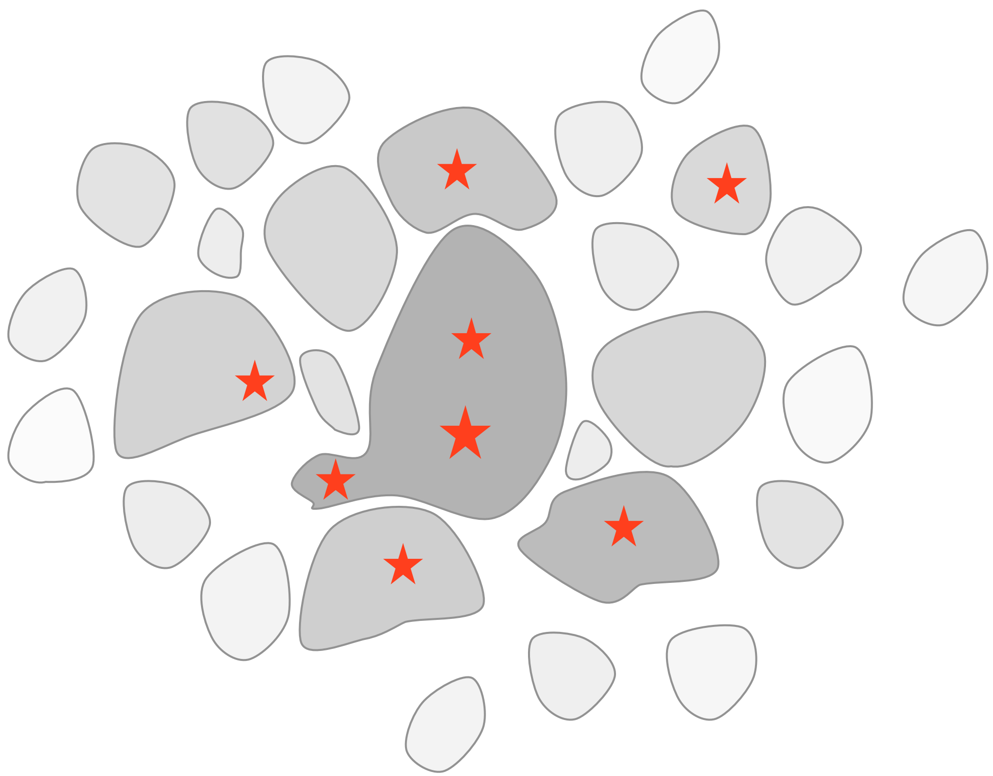


$\alpha = E_{kin}/|E_{pot}| < 1$

in *dense clusters*, clumps may merge while collapsing
--> then contain multiple protostars



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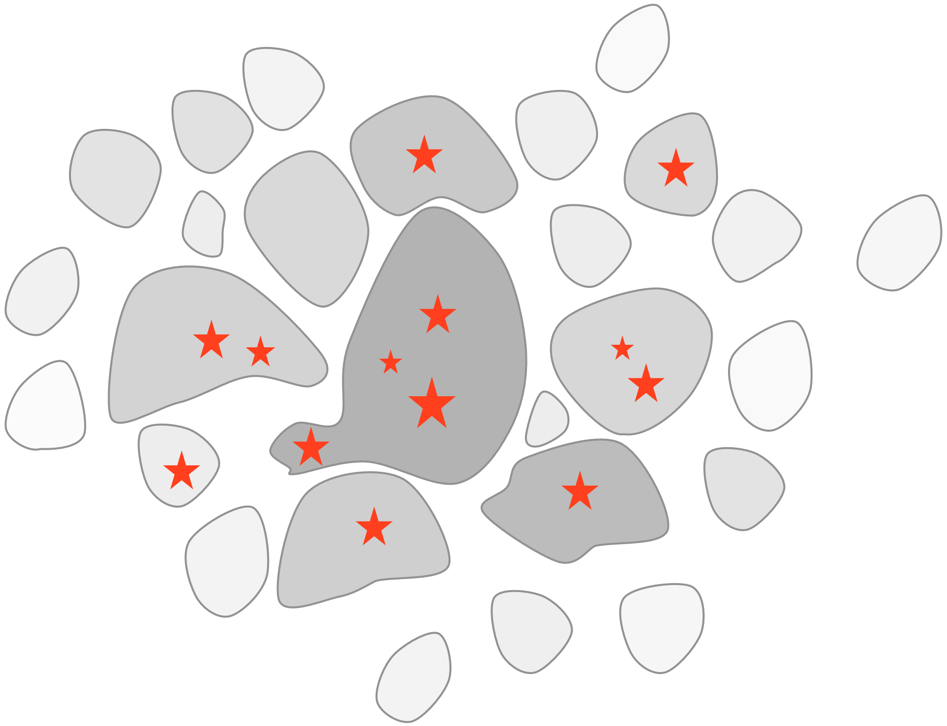

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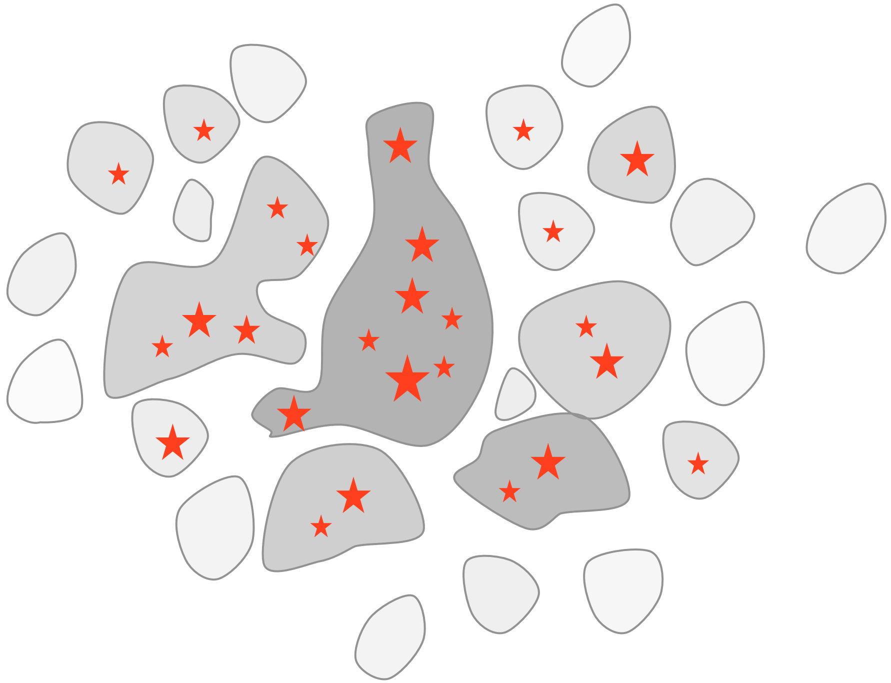
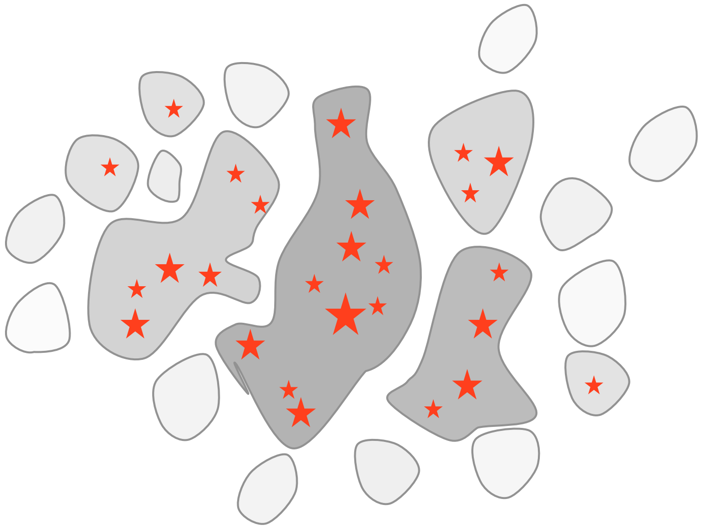


in *dense clusters*, competitive mass growth
becomes important



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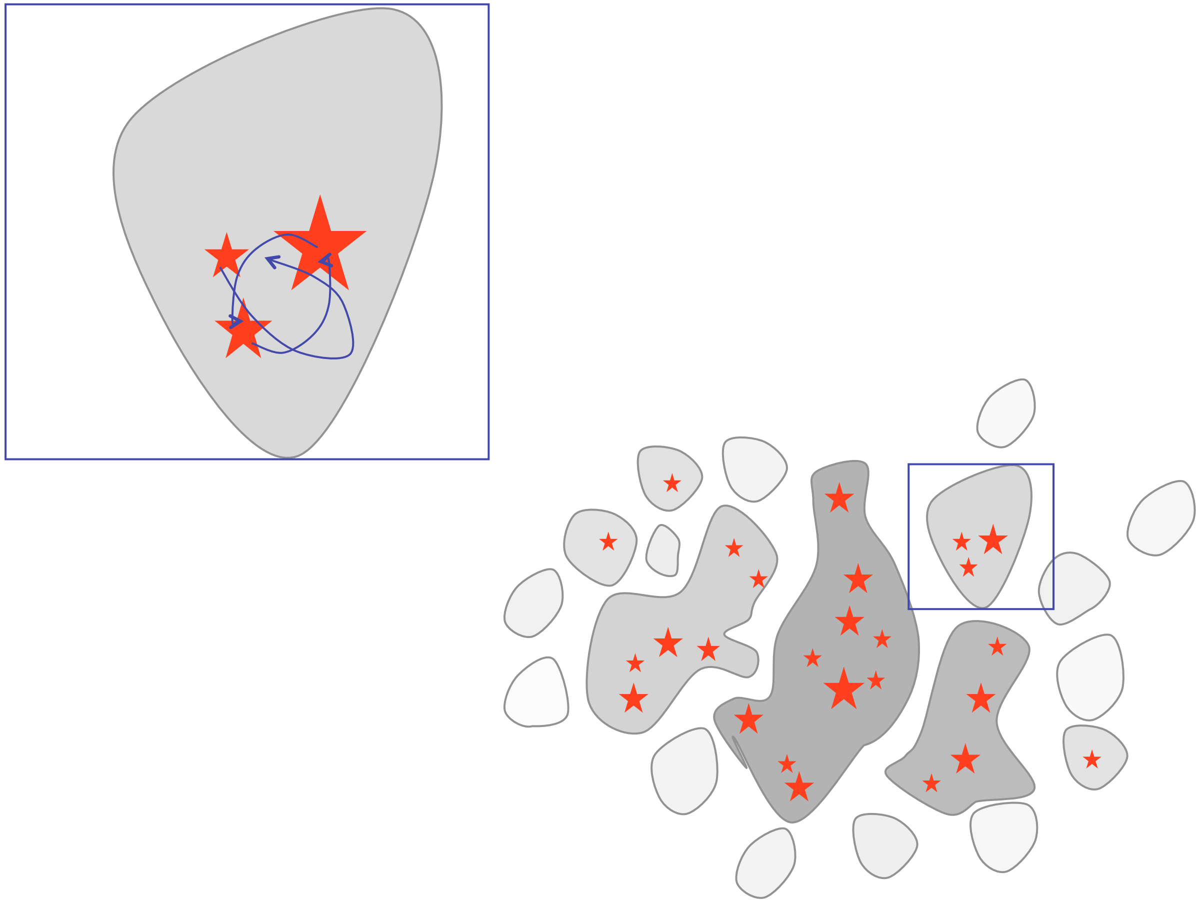
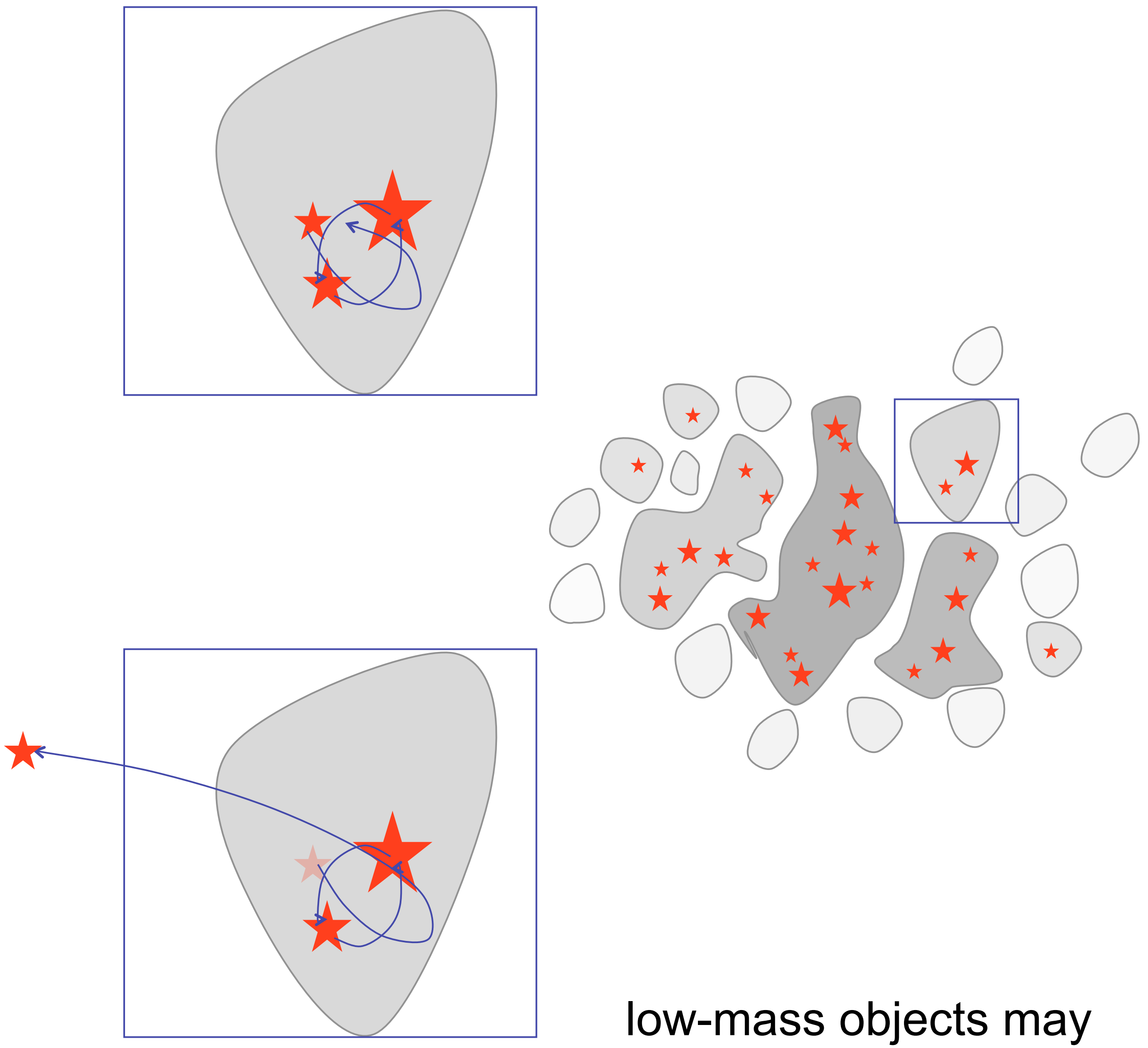
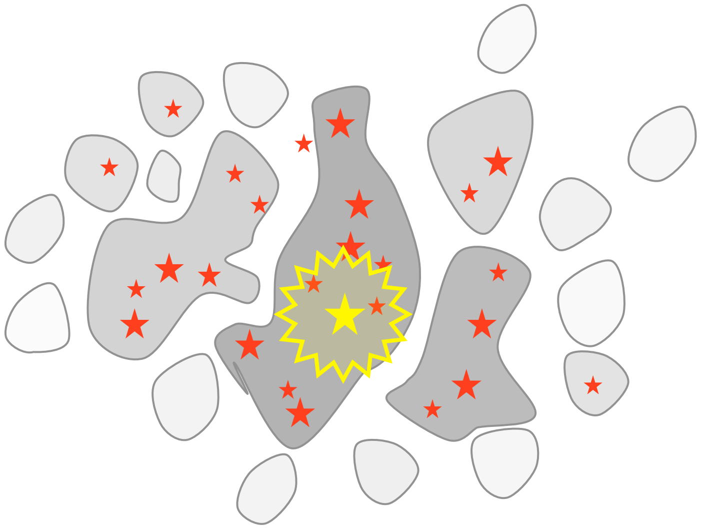


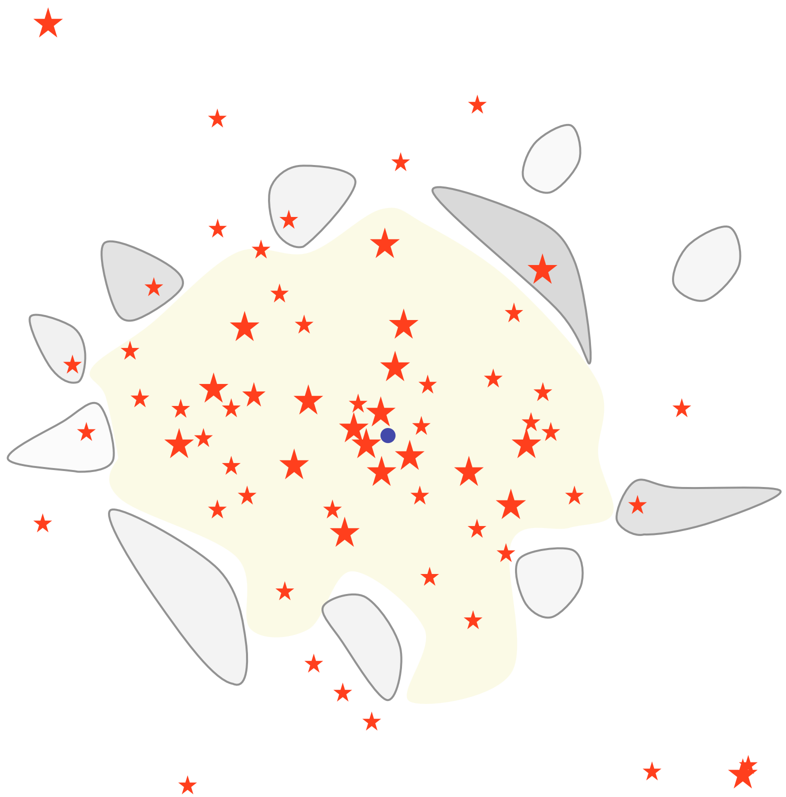
in *dense clusters*, *N*-body effects influence mass growth



low-mass objects may
become ejected --> accretion stops



feedback terminates star formation



result: *star cluster*, possibly with HII region