






Improving the basic ISM model

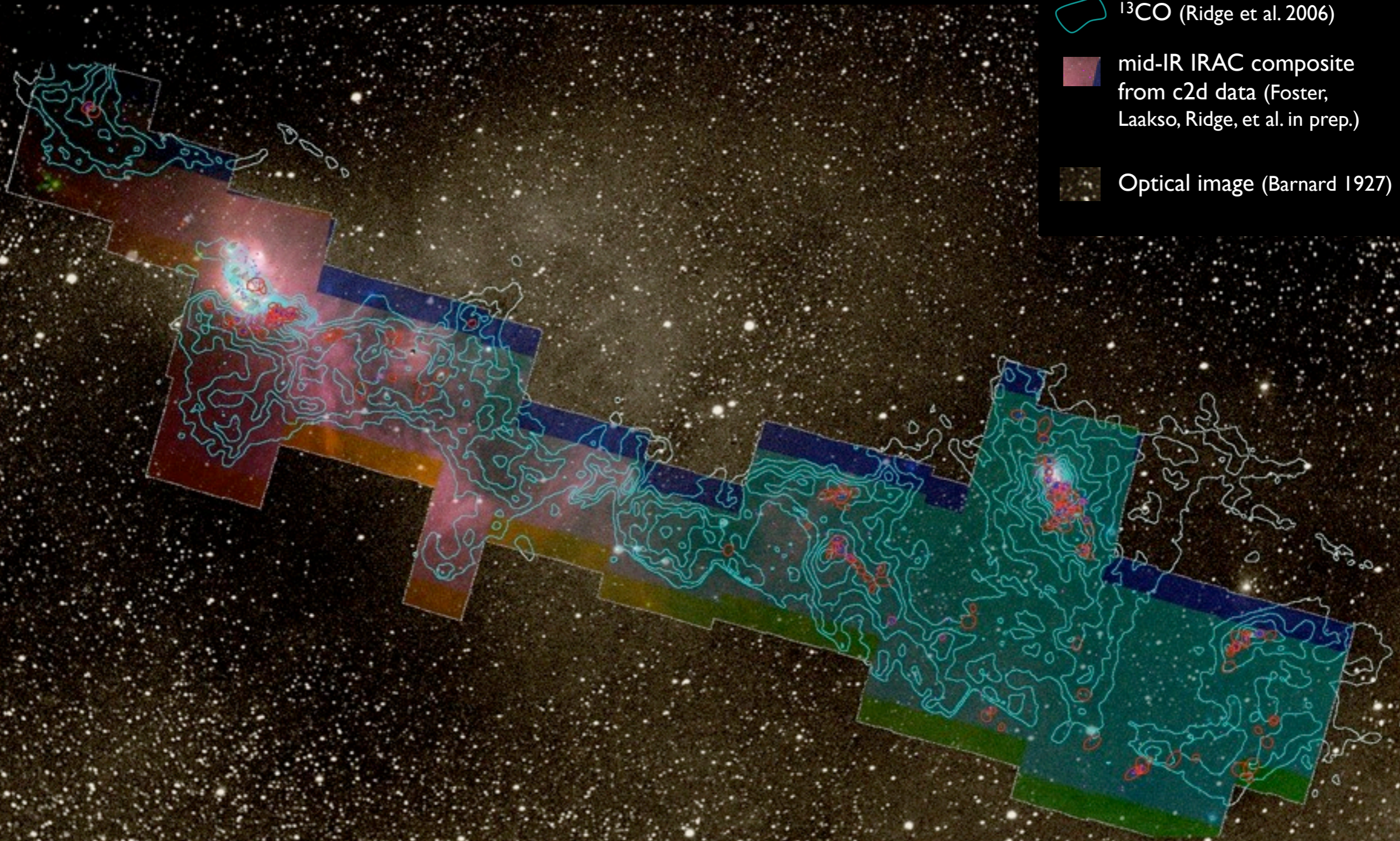
(some bells and whistles...)

CO as a tracer of cold dense gas

- Although we are interested in H_2 from a theoretical viewpoint, it's not what we observe.
- First energy-level of H_2 sits at a high temperature (512K), and so is not excited in the cold (well shielded) regions where H_2 forms.
- As such, we tend to resort to the next most abundant molecule, CO.
- Has a low energy transition (5.35 K), and is thus easily excited inside molecular clouds.
- Shown to be an excellent tracer of dense, cold gas






COMPLETE Perseus

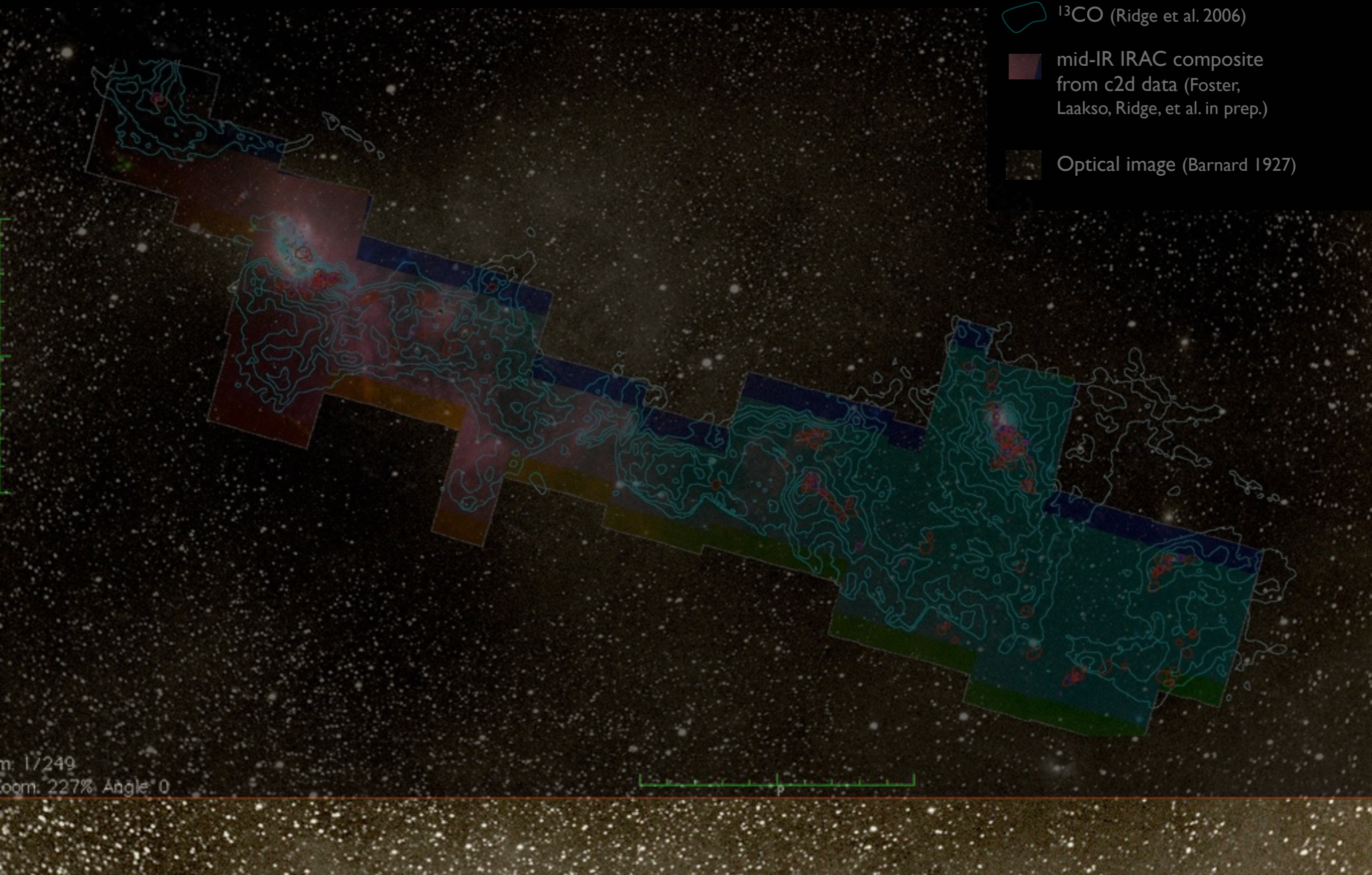
-  mm peak (Enoch et al. 2006)
-  sub-mm peak (Hatchell et al. 2005, Kirk et al. 2006)
-  ^{13}CO (Ridge et al. 2006)
-  mid-IR IRAC composite from c2d data (Foster, Laakso, Ridge, et al. in prep.)
-  Optical image (Barnard 1927)



COMPLETE Perseus






Image size: 1305 x 733
WL: 63 WW: 127

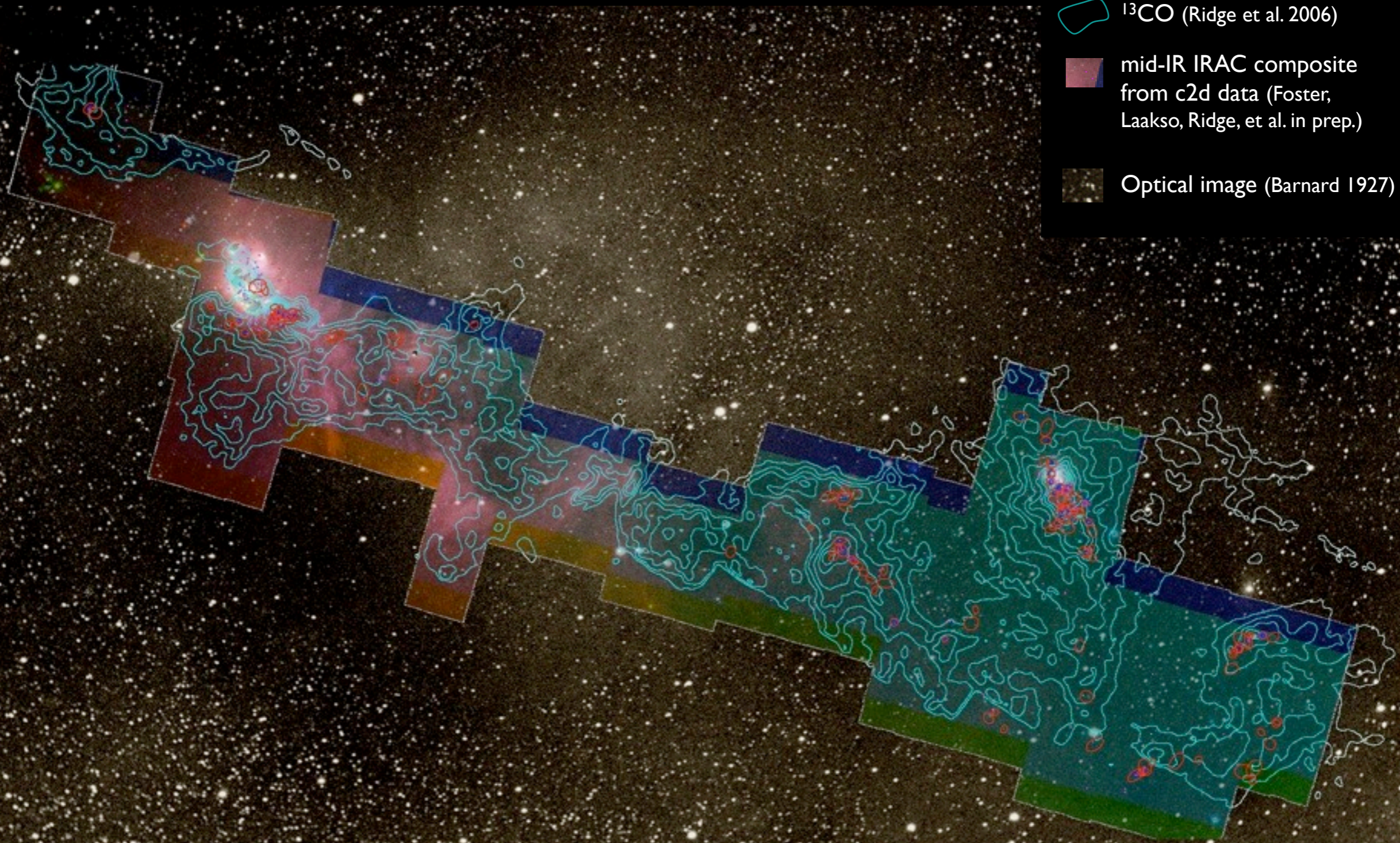
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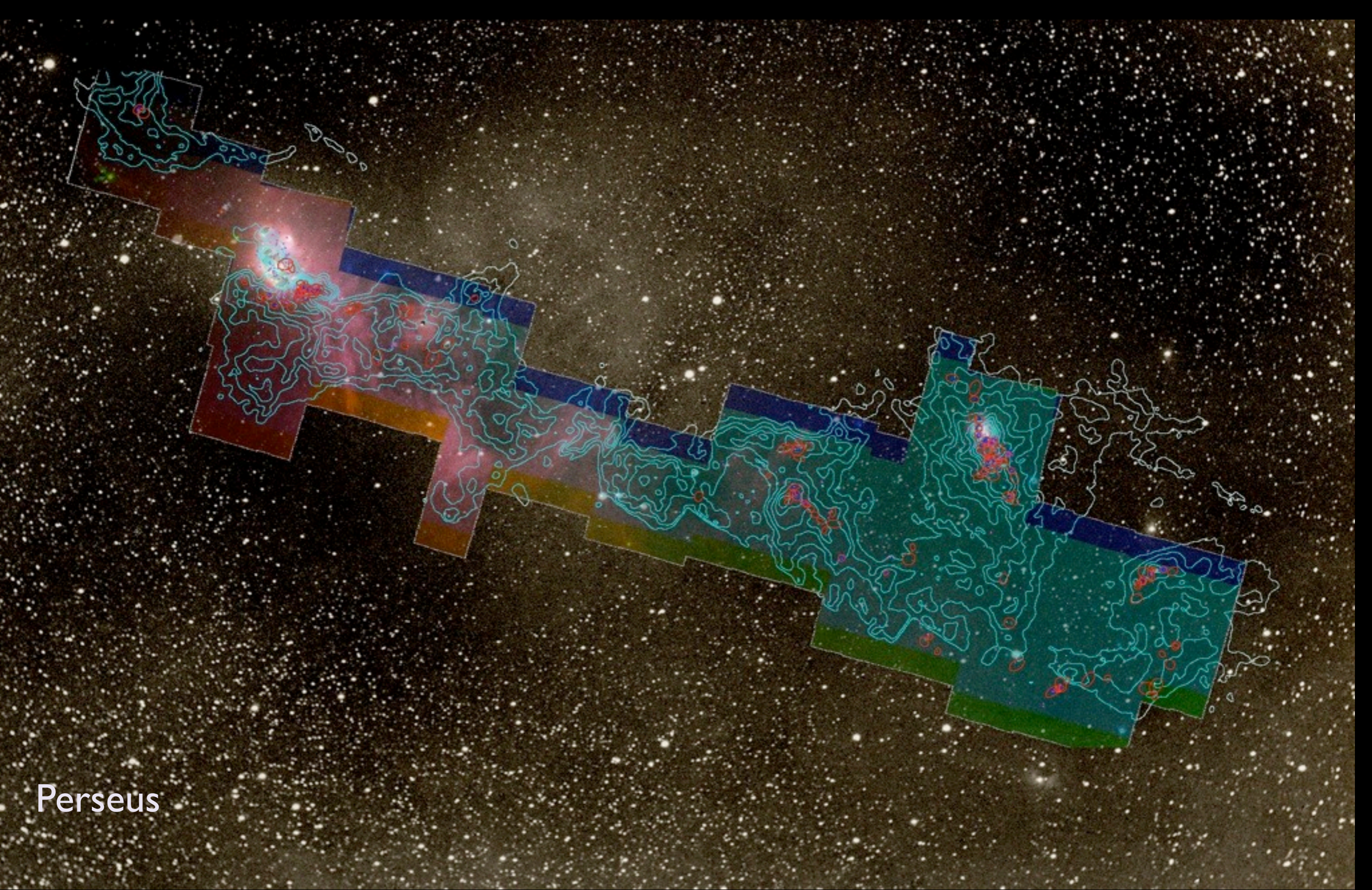


m: 1/249
Zoom: 227% Angle: 0

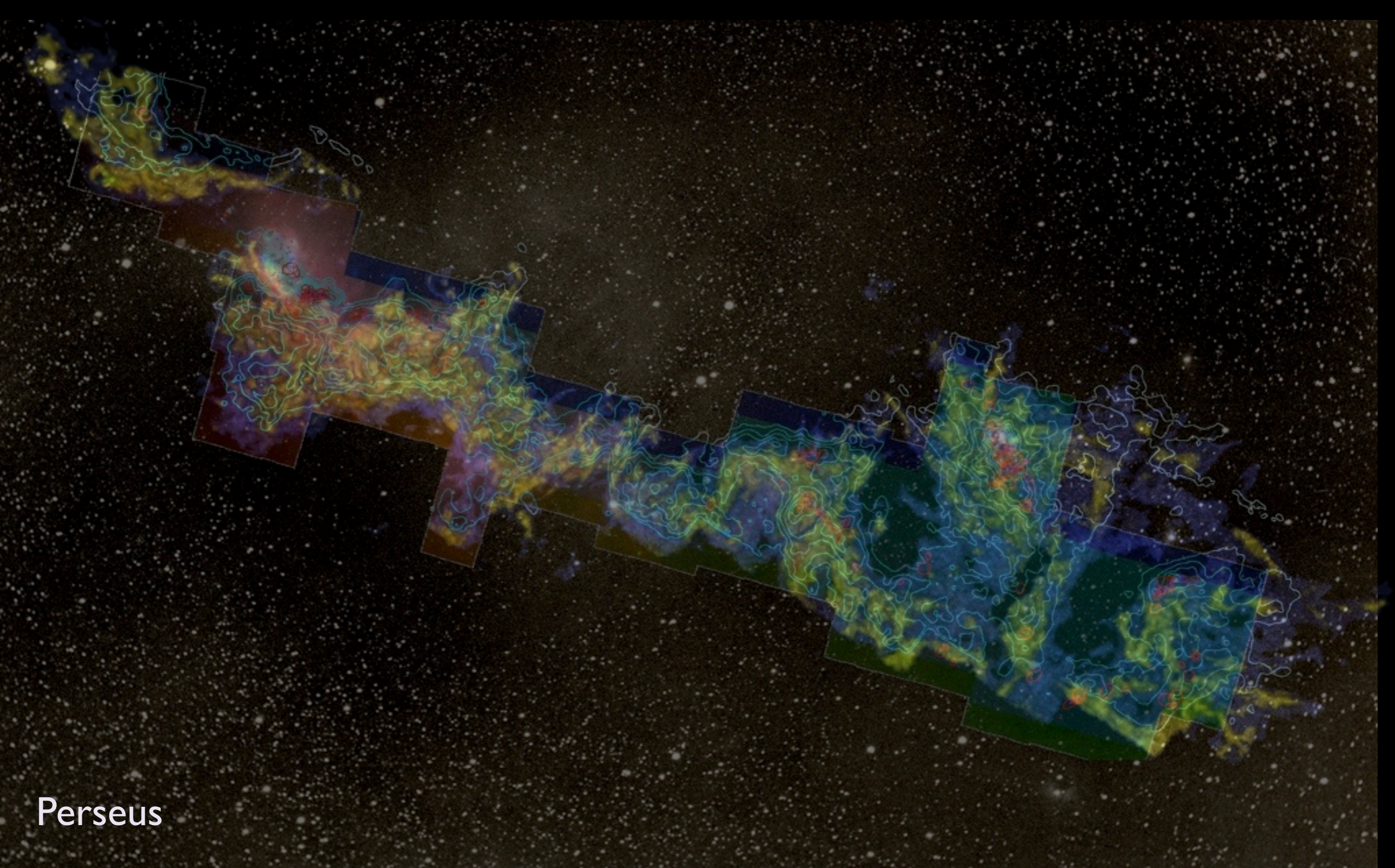
COMPLETE Perseus

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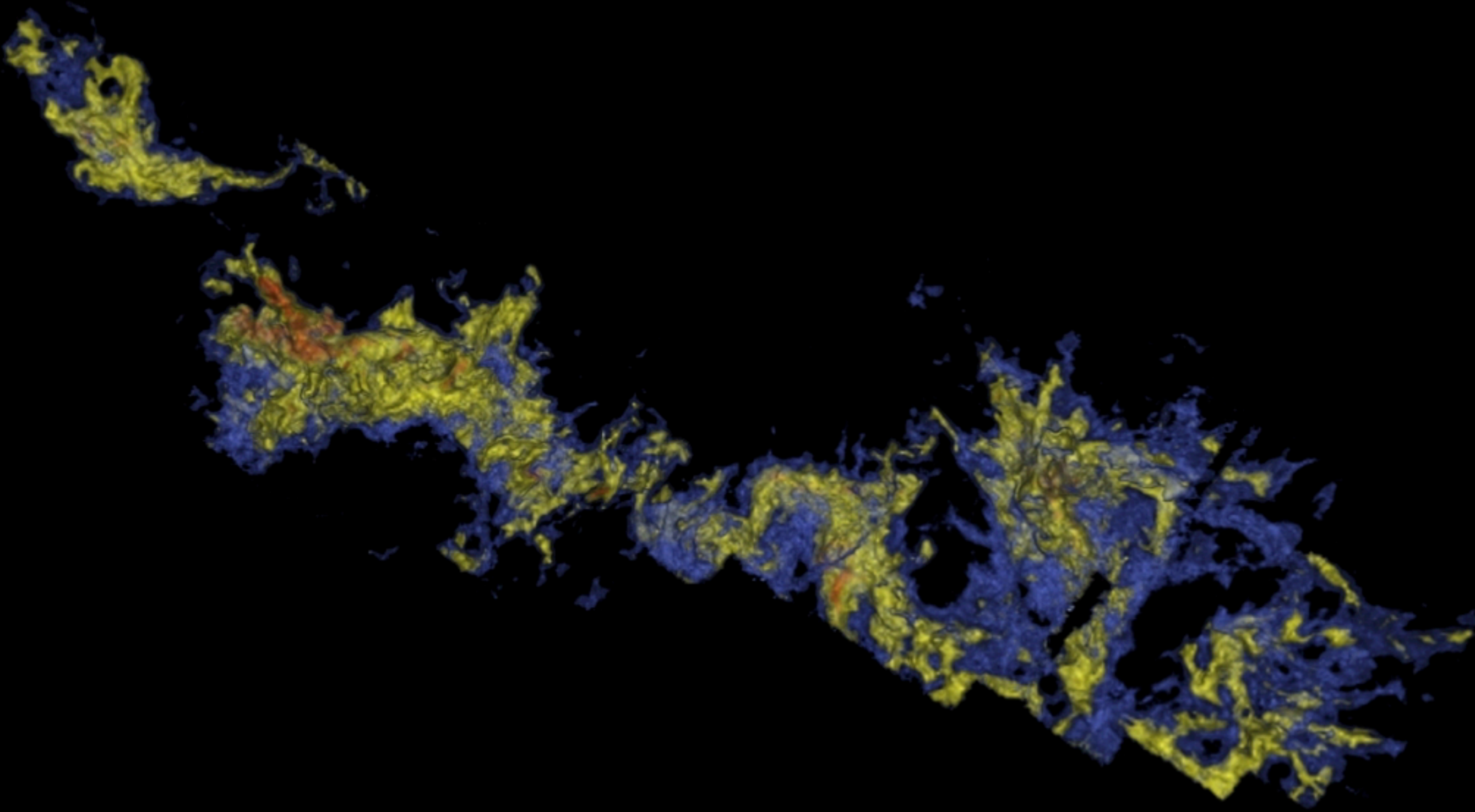


Perseus



Perseus

3D Viz made with VoView

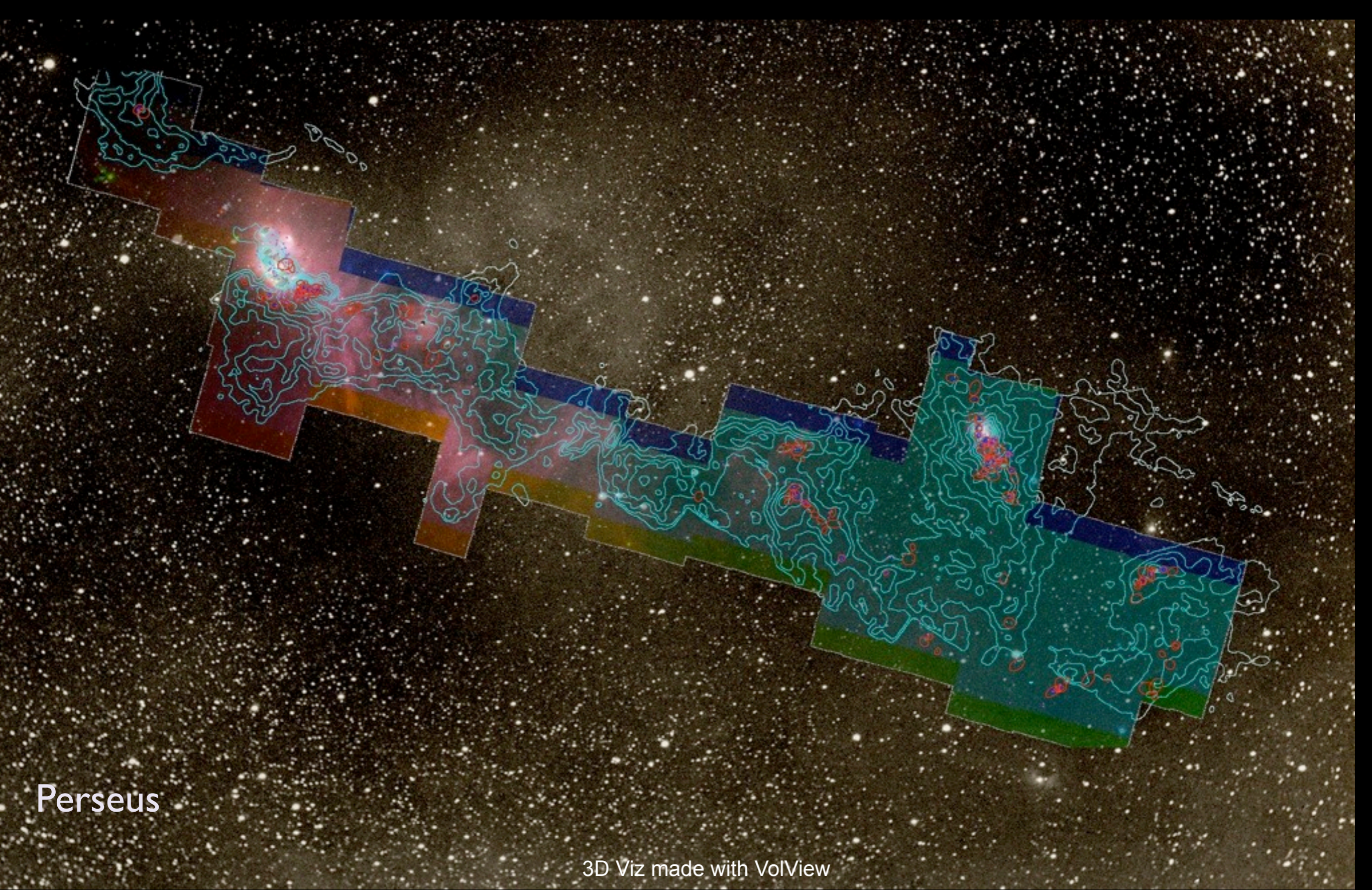


Perseus

3D Viz made with VolView

Astronomical **Medicine** **iig**

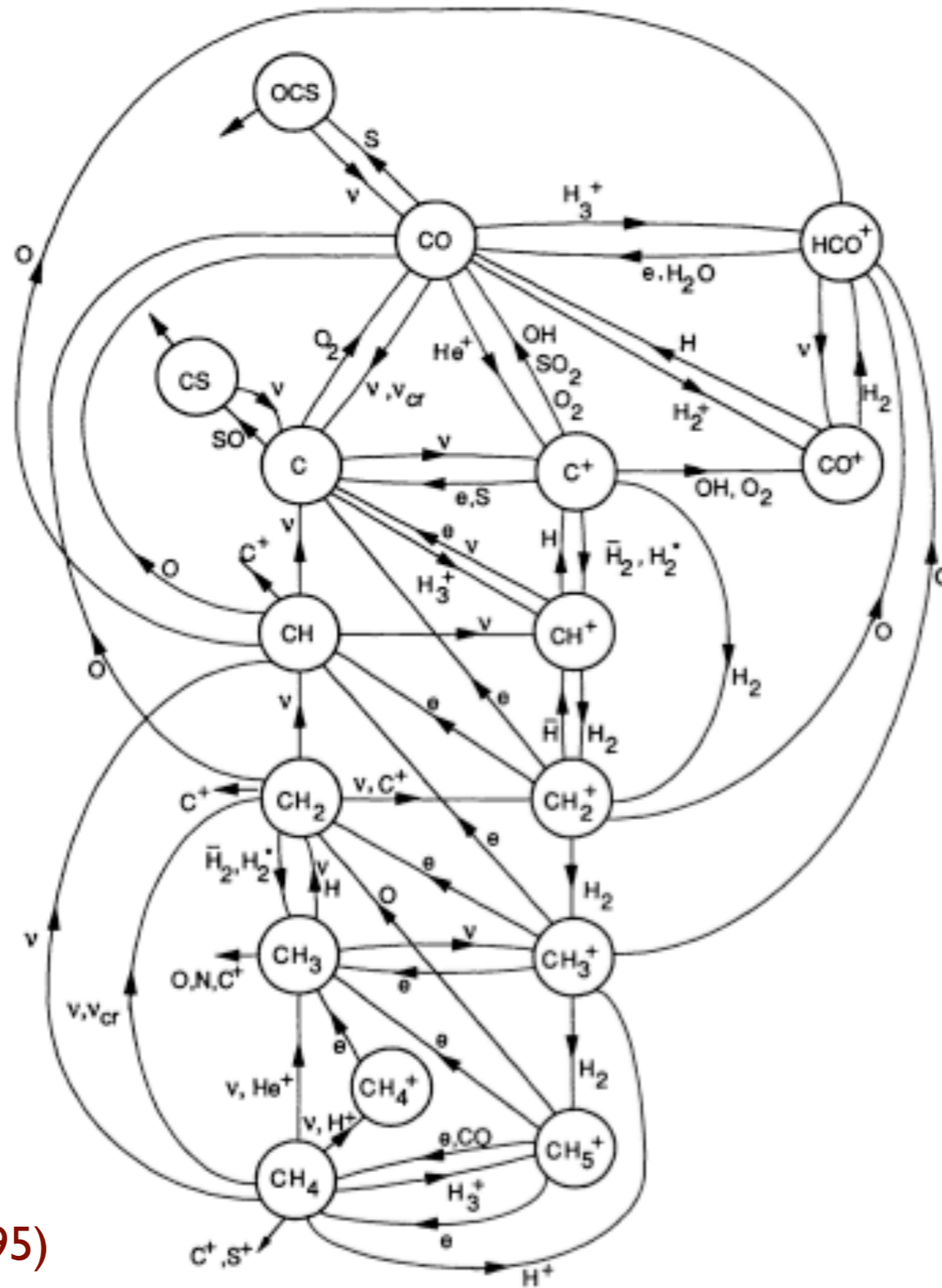
COMPLETE



Perseus

3D Viz made with VoView

CO chemistry



Sternberg & Dalgarno (1995)

Approximate CO chemistry

Nelson & Langer (1997):

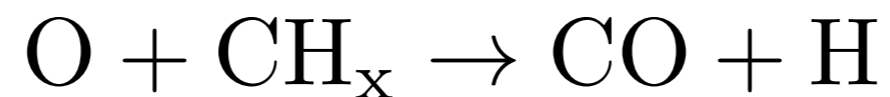
- Assumes that H is already in form of H₂
- Focus on the conversion of C⁺ ↔ CO
- Assume that reaction is initiated by the formation of a hydrocarbon radical (e.g. CH or CH₂) denoted as CH_x
- These are formed by slow radiative association reactions, eg:



- Taken to be the **rate-limiting step**

Nelson & Langer (1997):

- Intermediate CH_x ion or radical can then react to form CO:



- However not all the CH_x will get the chance to react -- some will be dissociated.
- NL97 express this with the ratio β :

$$\beta = \frac{k_1 x_{\text{O}}}{k_1 x_{\text{O}} + \Gamma_{\text{CH}_x} / n}$$

Approximate CO chemistry

Nelson & Langer (1997):

- Once CO has formed, they assume it is only destroyed via photodissociation, to form C and O.
- Also assume that C is instantly photo-ionised to C⁺ (no treatment of neutral C)
- The CO rate can then be written in the following format:

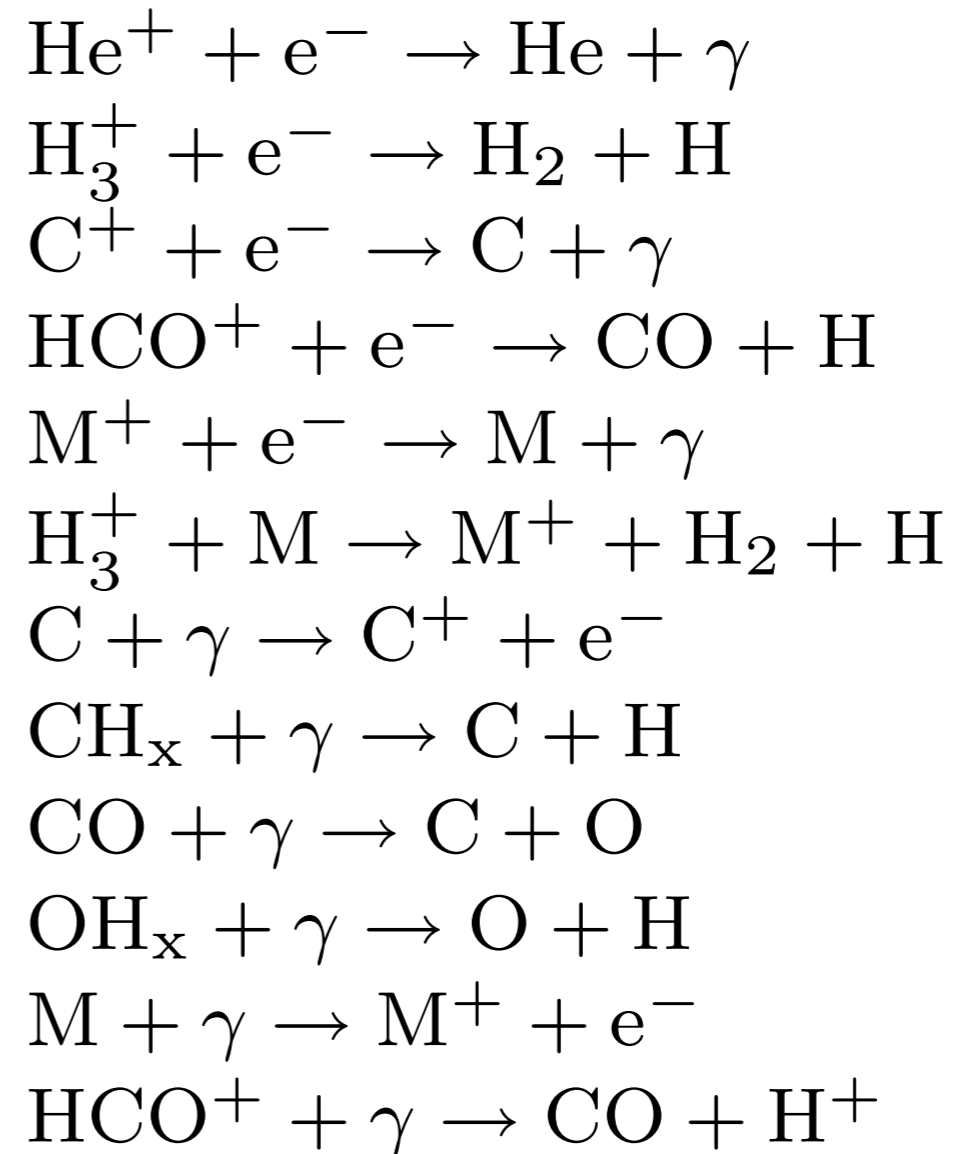
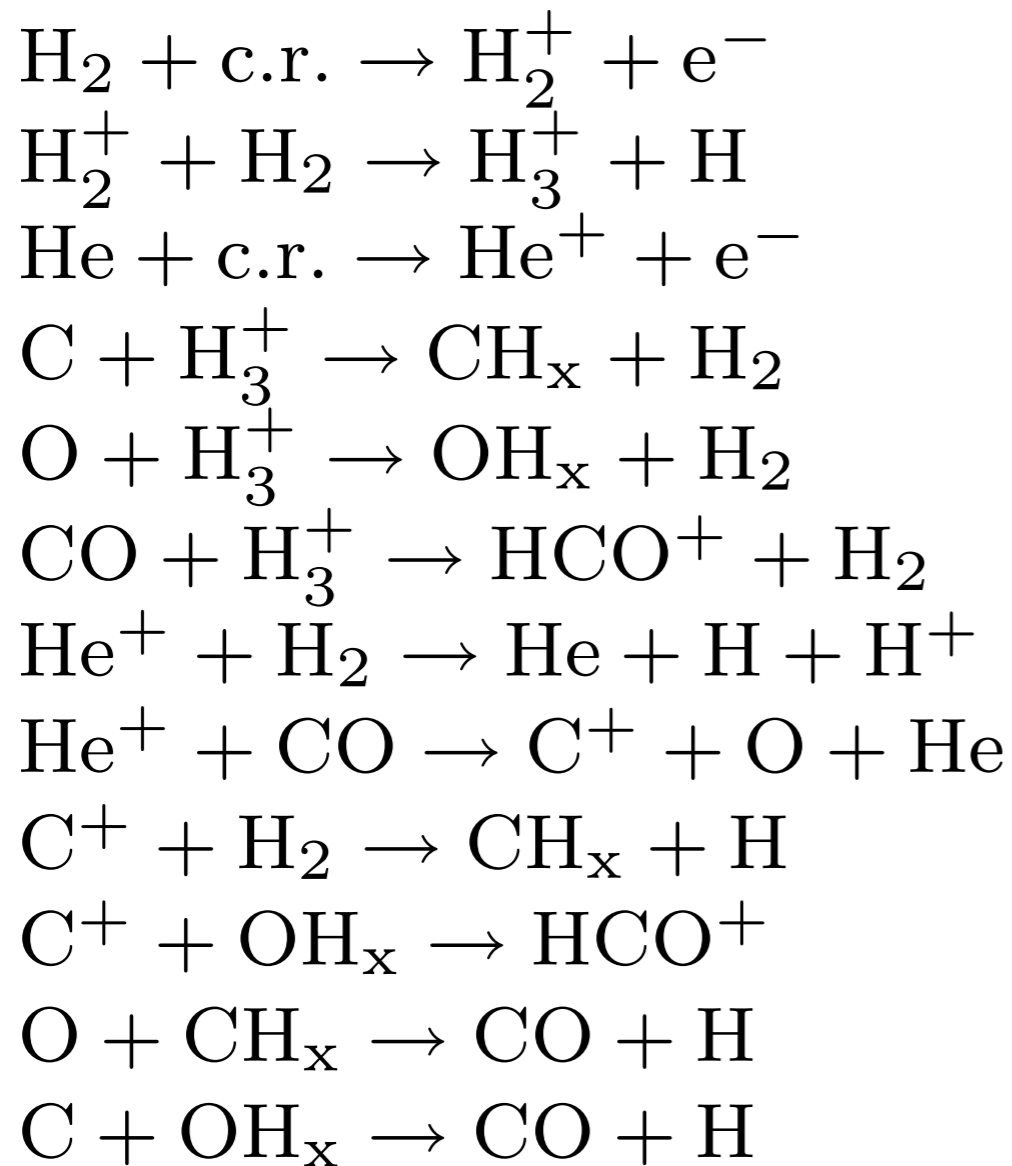
$$\frac{dn_{\text{CO}}}{dt} = k_0 n_{\text{C}^+} n_{\text{H}_2} \beta - \Gamma_{\text{CO}} n_{\text{CO}}$$

$$\Gamma_{\text{CO}} = 10^{-10} G_0 \exp(-2.5 A_V) \text{ s}^{-1} \quad \beta = \frac{k_1 x_{\text{O}}}{k_1 x_{\text{O}} + \Gamma_{\text{CH}_x}/n}$$

- The rate co-effs k_0 and k_1 are given by $5 \times 10^{-16} \text{ cm}^3/\text{s}$ and $5 \times 10^{-10} \text{ cm}^3/\text{s}$ respectively

Approximate CO chemistry

Nelson & Langer (1999):



Approximate CO chemistry

Glover et al. (2010):

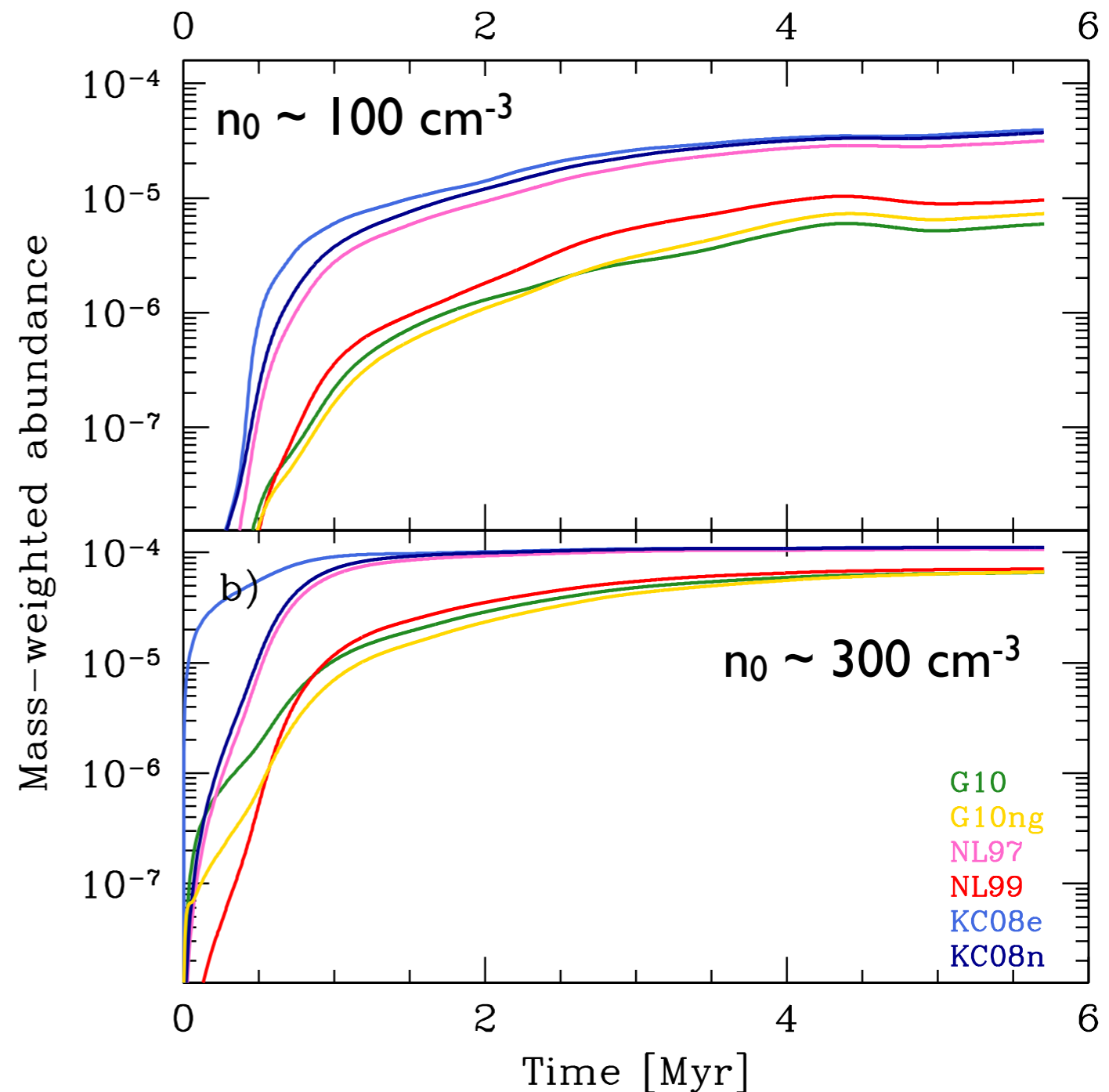
- 218 reactions with 32 species.
- Has recently been improved to include recombination of H^+ , He^+ and C^+ on the surface of dust grains.
- Yikes! Is this necessary?

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
93	$C_2 + He^+ \rightarrow C^+ + C + He$	$k_{93} = 1.6 \times 10^{-9}$	28
94	$OH + H^+ \rightarrow OH^+ + H$	$k_{94} = 2.1 \times 10^{-9}$	28
95	$OH + He^+ \rightarrow O^+ + He + H$	$k_{95} = 1.1 \times 10^{-9}$	28
96	$H_2O + H^+ \rightarrow H_2O^+ + H$	$k_{96} = 6.9 \times 10^{-9}$	64
97	$H_2O + He^+ \rightarrow OH + He + H^+$	$k_{97} = 2.04 \times 10^{-10}$	65
98	$H_2O + He^+ \rightarrow OH^+ + He + H$	$k_{98} = 2.86 \times 10^{-10}$	65
99	$H_2O + He^+ \rightarrow H_2O^+ + He$	$k_{99} = 6.05 \times 10^{-11}$	65
100	$O_2 + H^+ \rightarrow O_2^+ + H$	$k_{100} = 2.0 \times 10^{-9}$	64
101	$O_2 + He^+ \rightarrow O_2^+ + He$	$k_{101} = 3.3 \times 10^{-11}$	66
102	$O_2 + He^+ \rightarrow O^+ + O + He$	$k_{102} = 1.1 \times 10^{-9}$	66
103	$O_2^+ + C \rightarrow O_2 + C^+$	$k_{103} = 5.2 \times 10^{-11}$	28
104	$CO + He^+ \rightarrow C^+ + O + He$	$k_{104} = 1.4 \times 10^{-9} \left(\frac{T}{300}\right)^{-0.5}$	67
105	$CO + He^+ \rightarrow C + O^+ + He$	$k_{105} = 1.4 \times 10^{-16} \left(\frac{T}{300}\right)^{-0.5}$	67
106	$CO^+ + H \rightarrow CO + H^+$	$k_{106} = 7.5 \times 10^{-10}$	68
107	$C^- + H^+ \rightarrow C + H$	$k_{107} = 2.3 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	28
108	$O^- + H^+ \rightarrow O + H$	$k_{108} = 2.3 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	28
109	$He^+ + H^- \rightarrow He + H$	$k_{109} = 2.32 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.52} \exp\left(\frac{T}{22400}\right)$	69
110	$H_3^+ + e^- \rightarrow H_2 + H$	$k_{110} = 2.34 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.52}$	70
111	$H_3^+ + e^- \rightarrow H + H + H$	$k_{111} = 4.36 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.52}$	70
112	$CH^+ + e^- \rightarrow C + H$	$k_{112} = 7.0 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	71
113	$CH_2^+ + e^- \rightarrow CH + H$	$k_{113} = 1.6 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.6}$	72
114	$CH_2^+ + e^- \rightarrow C + H + H$	$k_{114} = 4.03 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.6}$	72
115	$CH_2^+ + e^- \rightarrow C + H_2$	$k_{115} = 7.68 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.6}$	72
116	$CH_3^+ + e^- \rightarrow CH_2 + H$	$k_{116} = 7.75 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	73
117	$CH_3^+ + e^- \rightarrow CH + H_2$	$k_{117} = 1.95 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	73
118	$CH_3^+ + e^- \rightarrow CH + H + H$	$k_{118} = 2.0 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.4}$	28
119	$OH^+ + e^- \rightarrow O + H$	$k_{119} = 6.3 \times 10^{-9} \left(\frac{T}{300}\right)^{-0.48}$	74
120	$H_2O^+ + e^- \rightarrow O + H + H$	$k_{120} = 3.05 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	75
121	$H_2O^+ + e^- \rightarrow O + H_2$	$k_{121} = 3.9 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	75
122	$H_2O^+ + e^- \rightarrow OH + H$	$k_{122} = 8.6 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	75
123	$H_3O^+ + e^- \rightarrow H + H_2O$	$k_{123} = 1.08 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	76
124	$H_3O^+ + e^- \rightarrow OH + H_2$	$k_{124} = 6.02 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.5}$	76
125	$H_3O^+ + e^- \rightarrow OH + H + H$	$k_{125} = 2.58 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.5}$	76
126	$H_3O^+ + e^- \rightarrow O + H + H_2$	$k_{126} = 5.6 \times 10^{-9} \left(\frac{T}{300}\right)^{-0.5}$	76
127	$O_2^+ + e^- \rightarrow O + O$	$k_{127} = 1.95 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.7}$	77
128	$CO^+ + e^- \rightarrow C + O$	$k_{128} = 2.75 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.55}$	78
129	$HCO^+ + e^- \rightarrow CO + H$	$k_{129} = 2.76 \times 10^{-7} \left(\frac{T}{300}\right)^{-0.64}$	79
130	$HCO^+ + e^- \rightarrow OH + C$	$k_{130} = 2.4 \times 10^{-8} \left(\frac{T}{300}\right)^{-0.64}$	79
131	$HOC^+ + e^- \rightarrow CO + H$	$k_{131} = 1.1 \times 10^{-7} \left(\frac{T}{300}\right)^{-1.0}$	28
132	$H^- + C \rightarrow CH + e^-$	$k_{132} = 1.0 \times 10^{-9}$	28
133	$H^- + O \rightarrow OH + e^-$	$k_{133} = 1.0 \times 10^{-9}$	28
134	$H^- + OH \rightarrow H_2O + e^-$	$k_{134} = 1.0 \times 10^{-10}$	28
135	$C^- + H \rightarrow CH + e^-$	$k_{135} = 5.0 \times 10^{-10}$	28
136	$C^- + H_2 \rightarrow CH_2 + e^-$	$k_{136} = 1.0 \times 10^{-13}$	28
137	$C^- + O \rightarrow CO + e^-$	$k_{137} = 5.0 \times 10^{-10}$	28
138	$O^- + H \rightarrow OH + e^-$	$k_{138} = 5.0 \times 10^{-10}$	28
139	$O^- + H_2 \rightarrow H_2O + e^-$	$k_{139} = 7.0 \times 10^{-10}$	28
140	$O^- + C \rightarrow CO + e^-$	$k_{140} = 5.0 \times 10^{-10}$	28
141	$H_2 + H^+ \rightarrow H_3^+ + \gamma$	$k_{141} = 1.0 \times 10^{-16}$	80

Relative accuracy

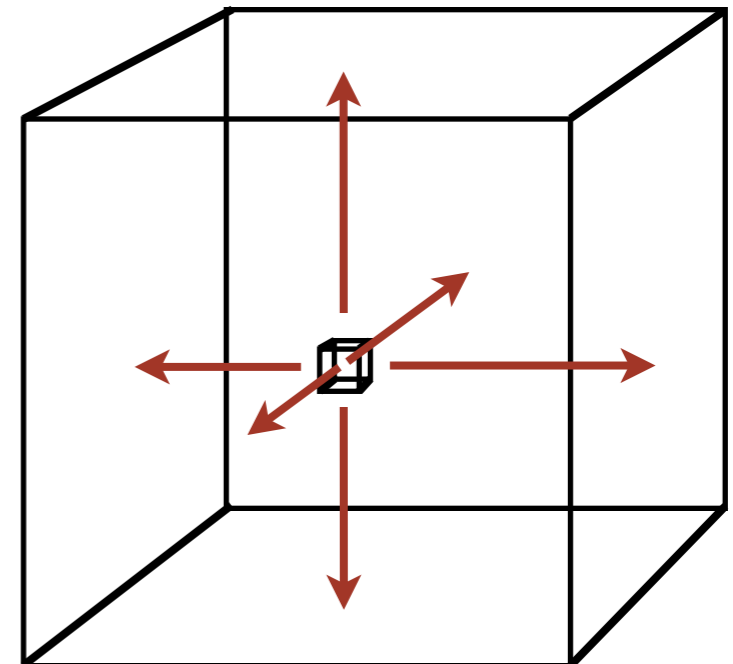
Glover & Clark (2012):

- NL97 tends to overestimate the CO by a factor of 2-3.
- Also tends to form too quickly
- But for galaxy-scale applications, it's not bad.
- NL99 is actually pretty good!
- This is also what Mark Krumholz uses in his DESPOTIC.

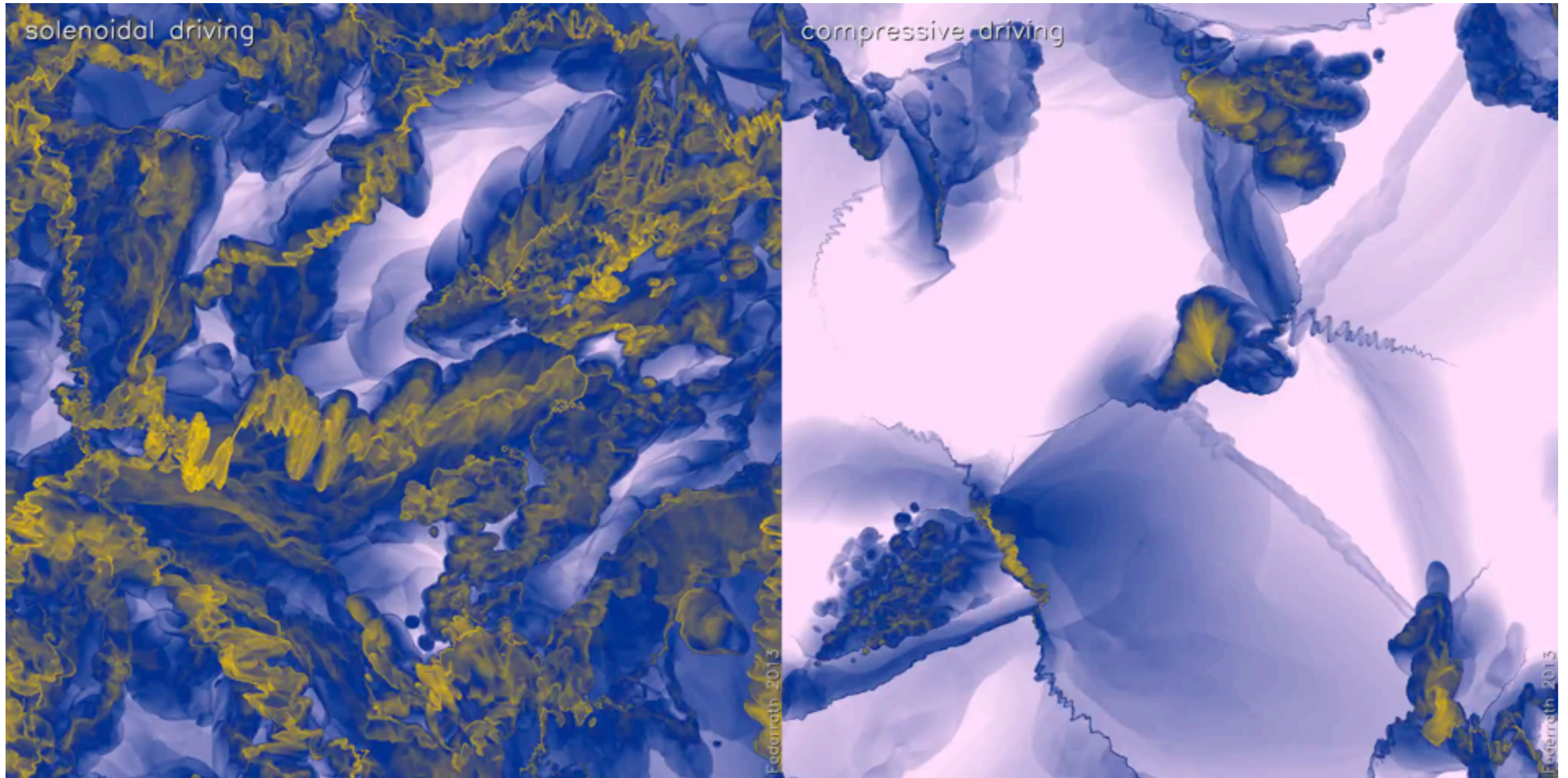


Improved shielding?

- Nelson & Langer (1997) also introduced the idea of '6 -ray'
- Basically, fire 6 rays along the cardinal axes of the simulation volume.
- Pretty cheap computationally.
- Also easy to parallelise
- Used in Glover & Mac Low (2007a,b) and Glover et al. (2010)

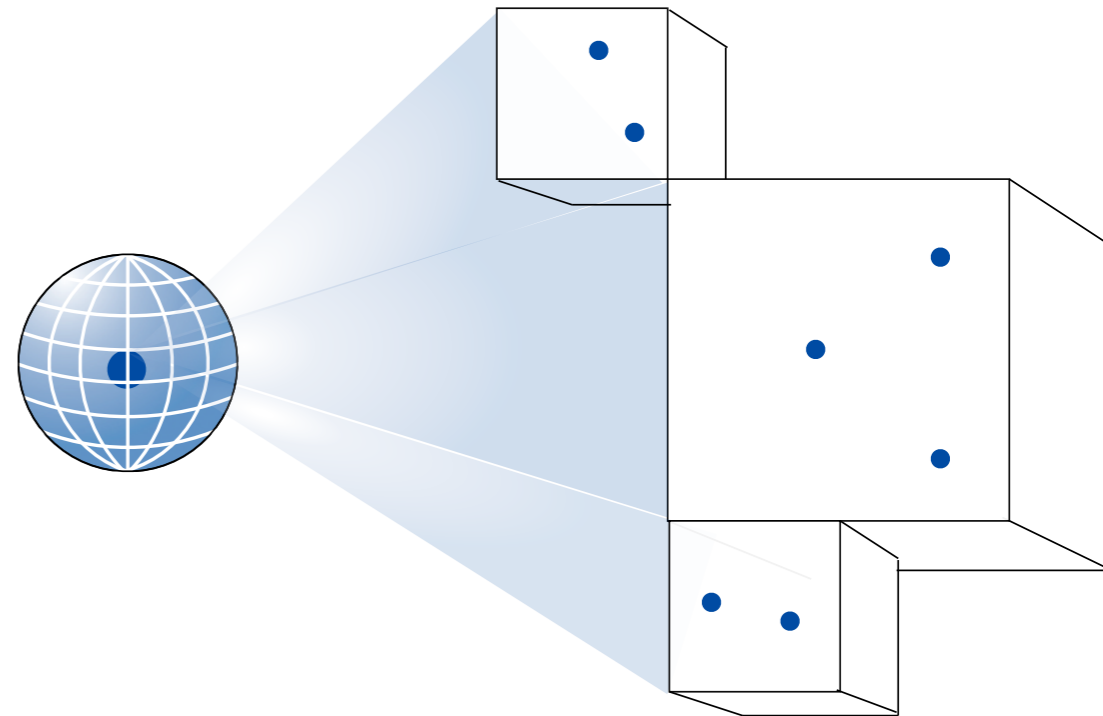


Depends on direction



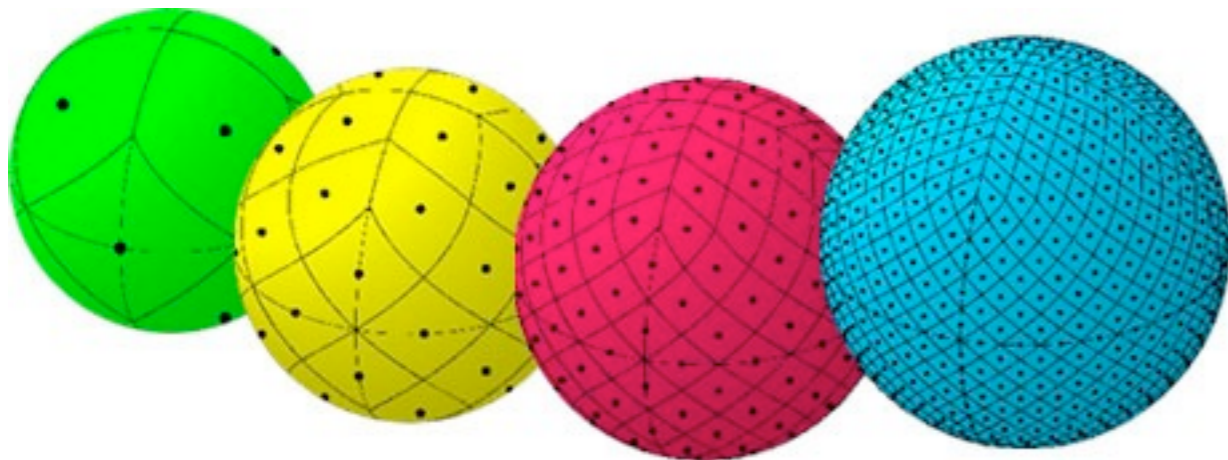
A better approach

- We came up with a new idea that uses the gravitational tree
- The tree contains information about how mass is distributed in the sky, as seen by the particle walking the tree.
- Tree gravity requires an opening angle -- so distance to the node, and the node's physical extent are stored.
- It also requires the node's mass and relative position.
- So we can work out the column density of the node, where it sits, and how much of the sky it takes up (solid angle)



How to store map?

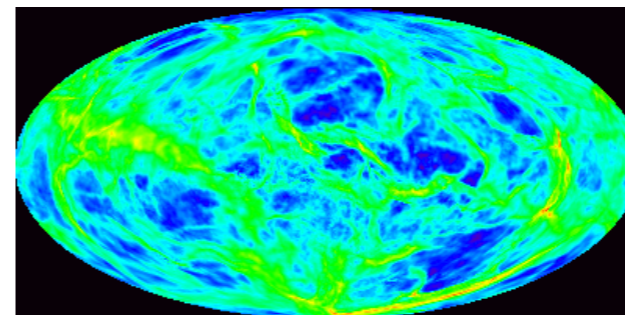
- We used the HEALPix algorithm (Górski et al. 2005)
- Equal area pixels



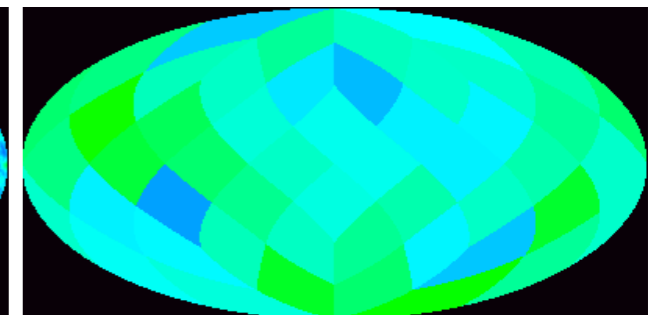
<http://healpix.jpl.nasa.gov>

Clark, Glover & Klessen (2012)

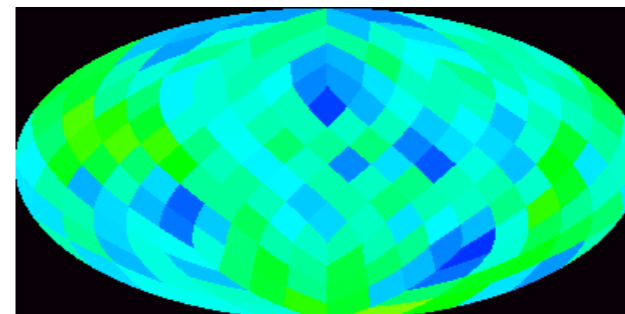
Full SPH particle map



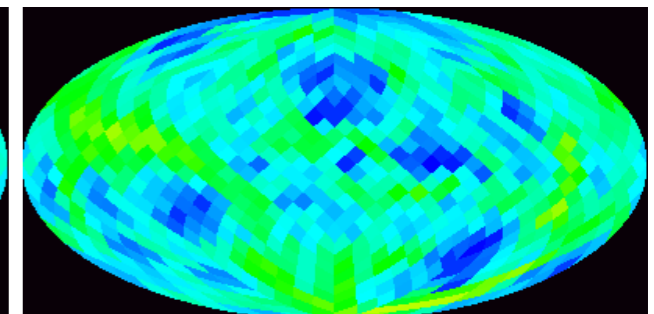
48 Healpix pixels



192 Healpix pixels



768 Healpix pixels

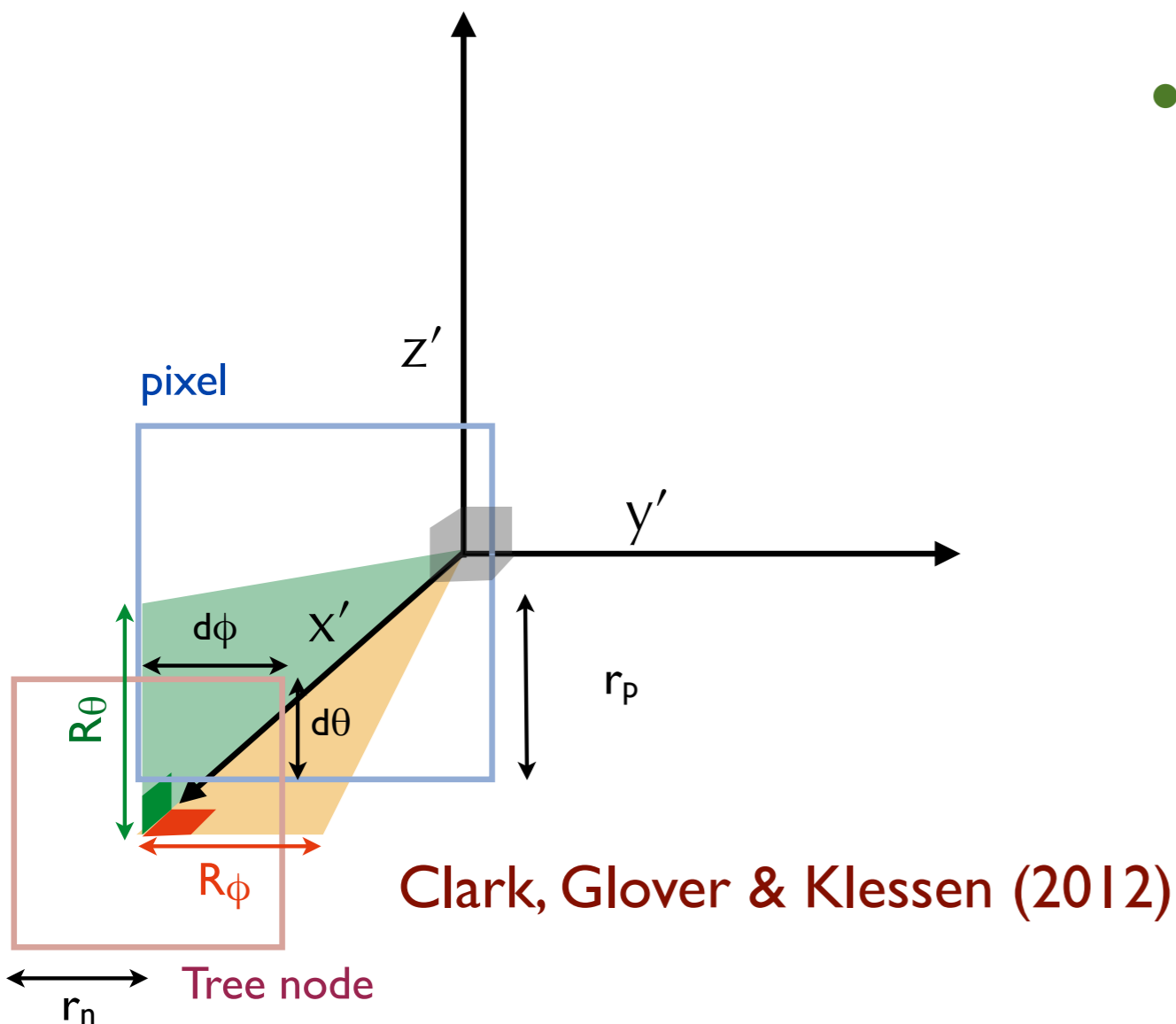


0.01 0.10
column density [g cm⁻²]

Mapping node to pixels

- **Problem:**

- The pixels have strange (diamond-like shapes)
- Nodes will be viewed from a random position



- **Solution:**

- Ignore this! Treat everything as squares on the sky!
- Rotate each pixel to frame tree node sits at

$$\mathbf{x} = (1, 0, 0)$$

Performance / accuracy

- Accuracy of algorithm in code paper is typically better than 10%
- Richard Wunsch pointed out that code paper version doesn't conserve mass.
- Suggested a simple re-normalisation step to ensure mass spread over pixels = mass in node.
- Achieves an accuracy of around a few percent for “standard” tree-opening angles.
- Note that accuracy will depend on the accuracy of the walk (i.e. the opening criteria).
- Also depends on the resolution of the map (we typically use 48 pixels).

Advantages

- Naturally adaptive.
- Easy to parallelise -- it's already been done for you!
- Relatively easy to implement (provided you know roughly how the tree works).
- Typically doubles the cost of the gravity walk.
- Doesn't need to be done each timestep! (essentially becomes 'free')
- Can be used to compute different quantities (total column, H2 column, velocities, optical depths, etc...)
- Has already been ported to several tree codes (Gadget2, Gadget3/ Arepo, FLASH)

Disadvantages

- Depending on how tree code is designed, it can be VERY memory hungry.
- In Gadget2/3 & Arepo the parallelised tree works by sending copies of local particle on one MPI thread to the other MPI threads to get the gravity contributions from the domain held by these threads.
- Need to send a copy of the map with the particle copy, AND keep a copy locally.
- In Gadget 2 we have 2 maps each for $\Sigma_{\text{H}_2} + \Sigma_{\text{CO}} + \Sigma_{\text{total}}$ so that's 6×48 real*4 variables *per particle*.
- In FLASH, things are different: MPI threads sent info **to** the target thread.
- Only a handful of cells walking tree at any time: memory overhead is very small!

How to use the rays

- Chemistry + cooling/heating requires a single column (or A_V) which enters the rate equations.
- Note that this is just a simple sum with the HEALPix scheme, as all the pixels extend the same solid angle.

So for basic 48 pixel resolution:

$$A_{V,\text{mean}} = -\frac{1}{2.5} \ln \left[\frac{1}{48} \sum_{i=1}^{48} \exp(-2.5 A_{V,i}) \right]$$

Calculating T_{dust}

- In the model you are using, the T_{dust} temperature is fixed.
- However we would ideally like to be able to calculate this self-consistently in the clouds
- Dust temperature is calculated by iterating the balance between the heating and cooling processes:

$$\Gamma_{\text{ext}} + \Gamma_{\text{H}_2} + \Gamma_{\text{G-D}} + \Lambda_{\text{Dust}} = 0$$

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Heating due to
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the ISRF

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Heating from H_2 formation on grain surfaces

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Heating due to absorption of the ISRF

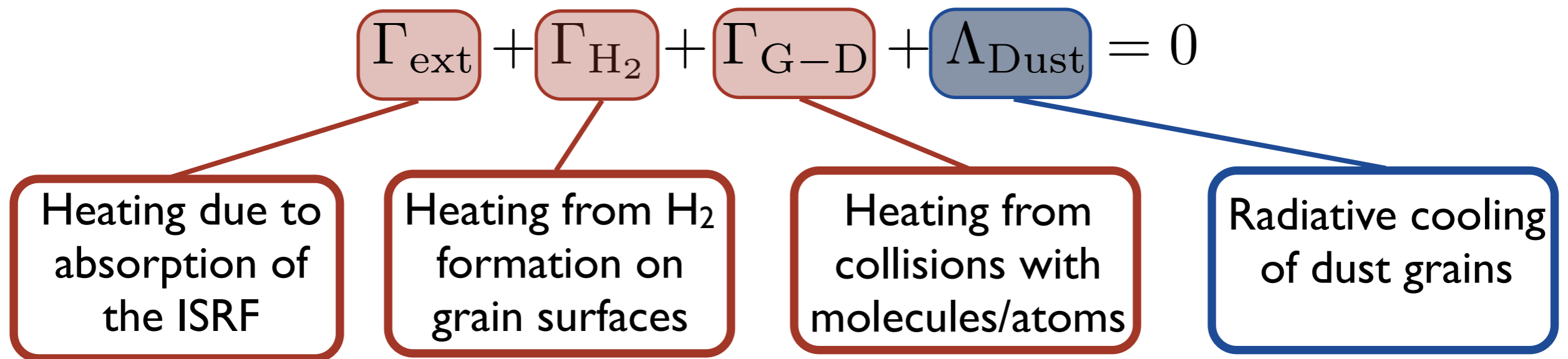
Heating from H_2 formation on grain surfaces

Heating from collisions with molecules/atoms

Radiative cooling of dust grains

Calculating T_{dust}

- In the model you are using, the T_{dust} temperature is fixed.
- However we would ideally like to be able to calculate this self-consistently in the clouds
- Dust temperature is calculated by iterating the balance between the heating and cooling processes:



- Implicit assumption that the timescale associated with these changes is small compared to the other timesteps in the system.

Calculating τ_{dust}

- Following Goldsmith (2001), we can express Γ_{ext} as a function of the optically thin heating rate $\Gamma_{\text{ext},0}$ and an attenuation factor χ :

$$\Gamma_{\text{ext},0} = 4\pi D\rho \int_0^\infty J_\nu \kappa_\nu d\nu$$

$$\Gamma_{\text{ext}} = \chi \Gamma_{\text{ext},0}$$

$$\chi(N) = \frac{\int_0^\infty J_\nu \kappa_\nu \exp(-\kappa_\nu \Sigma) d\nu}{\int_0^\infty J_\nu \kappa_\nu d\nu}$$

- χ can be precomputed, and used as a lookup table.
- Compute average over the pixels (i.e. in 6-ray or TREECOL)
- Equivalent to doing the integration over all solid angles.

Calculating T_{dust}

- Dust cooling in the optically thin regime is pretty trivial:

$$\Lambda(T_{\text{dust}}) = 4\pi D\rho \int_0^\infty B_\nu(T_{\text{dust}}) \kappa_\nu d\nu$$

- We adopt a mixture opacities...
 - $\lambda > 1 \mu\text{m}$: Ossenkopf & Henning (1994) opacities (non-coagulated and thick ice-mantels).
 - $\lambda < 1 \mu\text{m}$: Mathis, Mezger & Panagia (1983)
- Then the above expression can be approximated as:

$$\Lambda(T_{\text{dust}}) \approx 4.7 \times 10^{-31} T_{\text{dust}}^6 n \text{ erg s}^{-1} \text{ cm}^{-3}$$

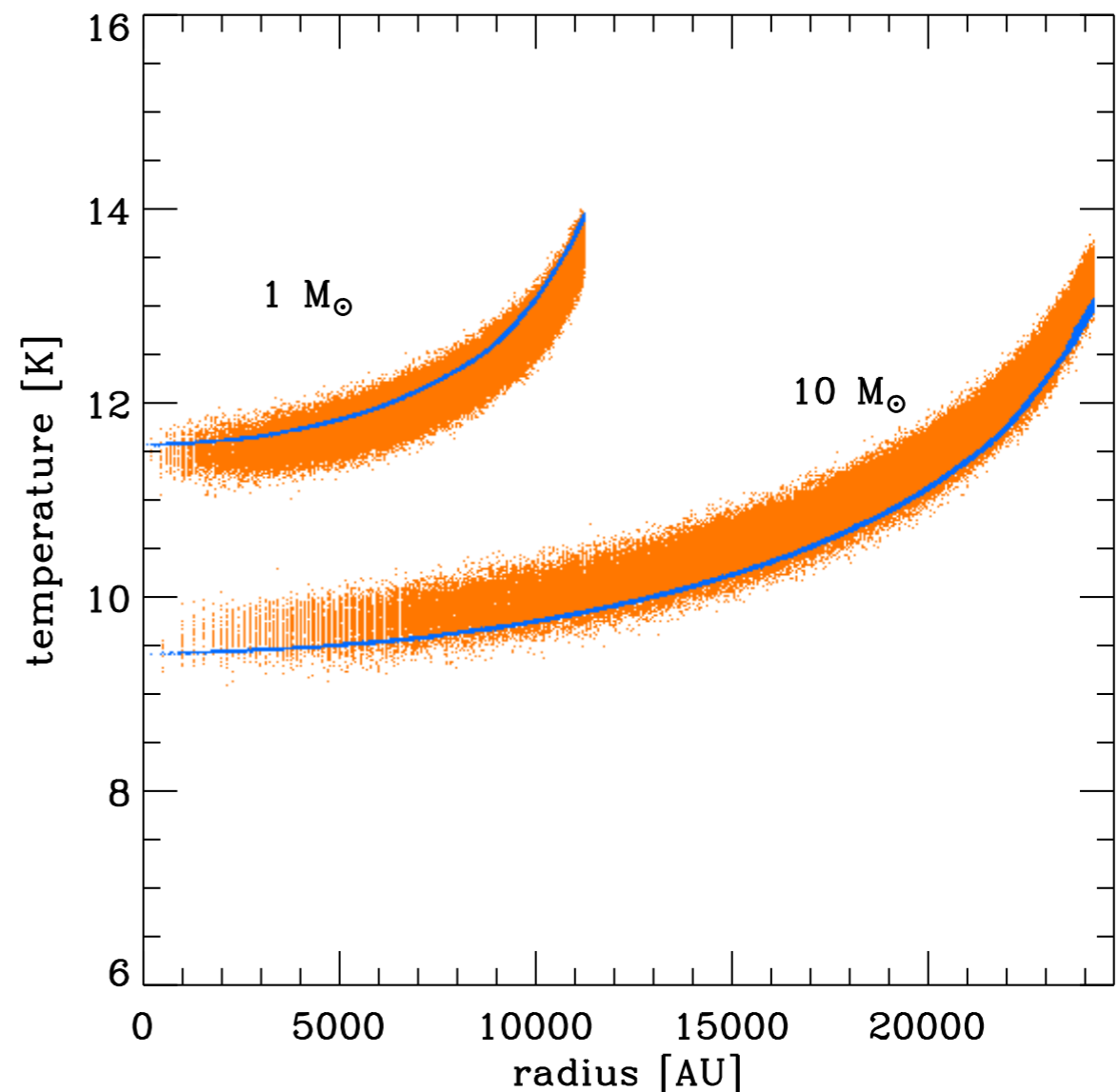
- Accurate to a few % in the range $5 < T_{\text{dust}} < 100 \text{ K}$

Calculating T_{dust}

- We have already discussed the gas-dust heat exchange $\Gamma_{\text{G-D}}$ -- just remember to change the sign!
- More uncertain is the heating rate of the dust due to H_2 formation!
- Excess energy is split between
 - Kinetic energy of the H_2 molecule
 - Internal energy levels of the H_2 molecule
 - The dust grain
- However, unless the background radiation field is very small, this typically is a small contribution (can ignore it if you wish).

How good is this simple estimate?

- Clark et al. 2012:
 - Compared the T_{dust} estimate from TreeCol + Goldsmith 2001 with Dullemond's RADMC-3D
 - Results are pretty good!
- Using the radiation field of Black (1994)
- $G_0 = 1.7$



Treating line cooling

Yoshida et al. 2006, ApJ, 652, 6:

$$\Lambda_{X,\text{thick}}(T) = \sum_{u,l} h\nu_{ul} \beta_{\text{esc},ul} A_{ul} n_{X,u}$$

$$\beta_{\text{esc},ul} = \frac{1 - \exp(-\tau_{ul})}{\tau_{ul}},$$

$$\tau_{ul} = \alpha_{ul} L_s$$

$$L_s = \frac{v_{\text{th}}}{|dv_r/dr|},$$

Treating line cooling

- Since the line absorption co-eff is linearly proportional to the number density of the species in interest, we can write the optical depth as,

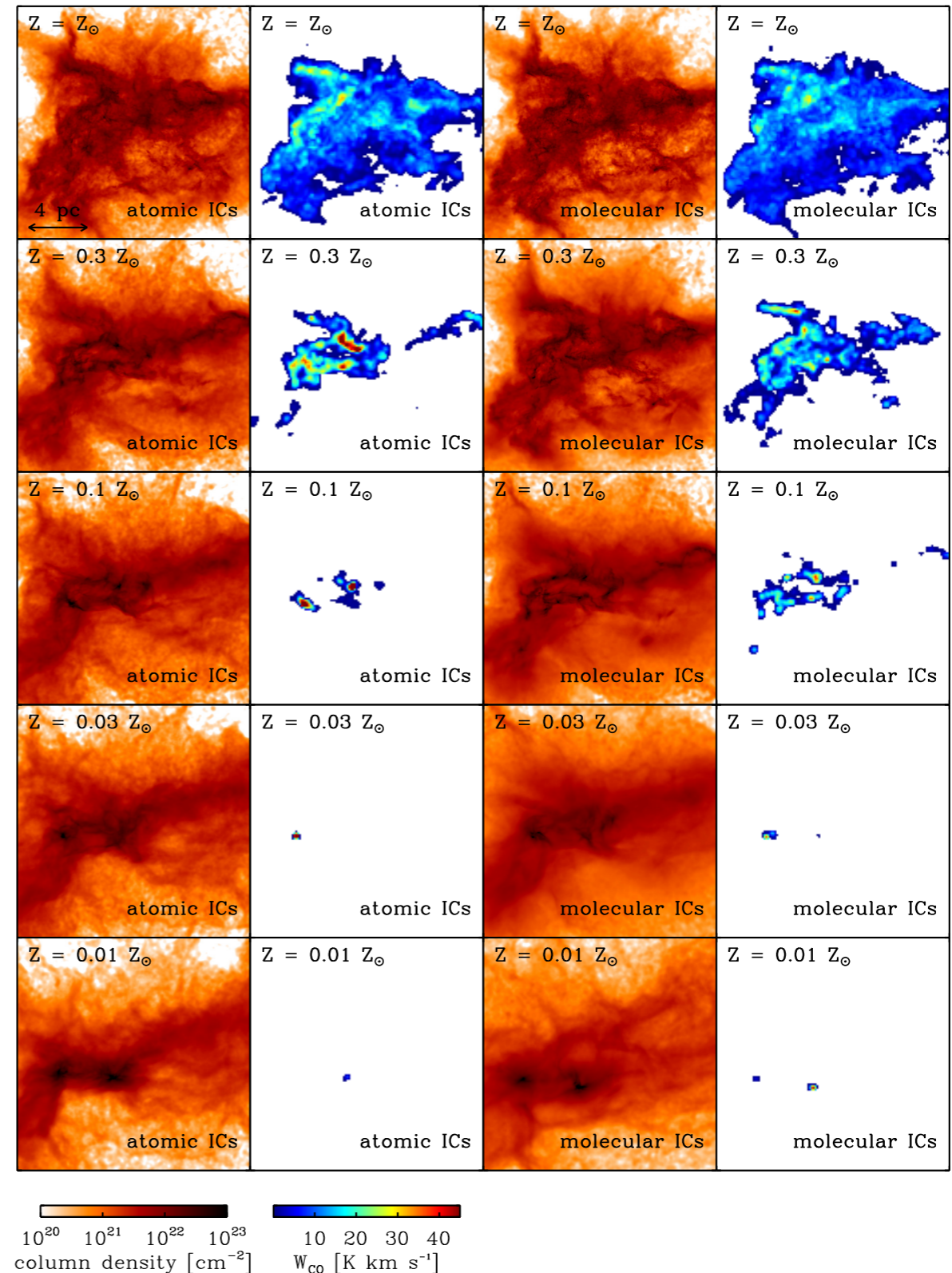
$$\tau_{ul} = \left(\frac{\alpha_{ul}}{n_X} \right) N_{X,\text{eff}}$$

where $N_X \equiv n_X L_s$

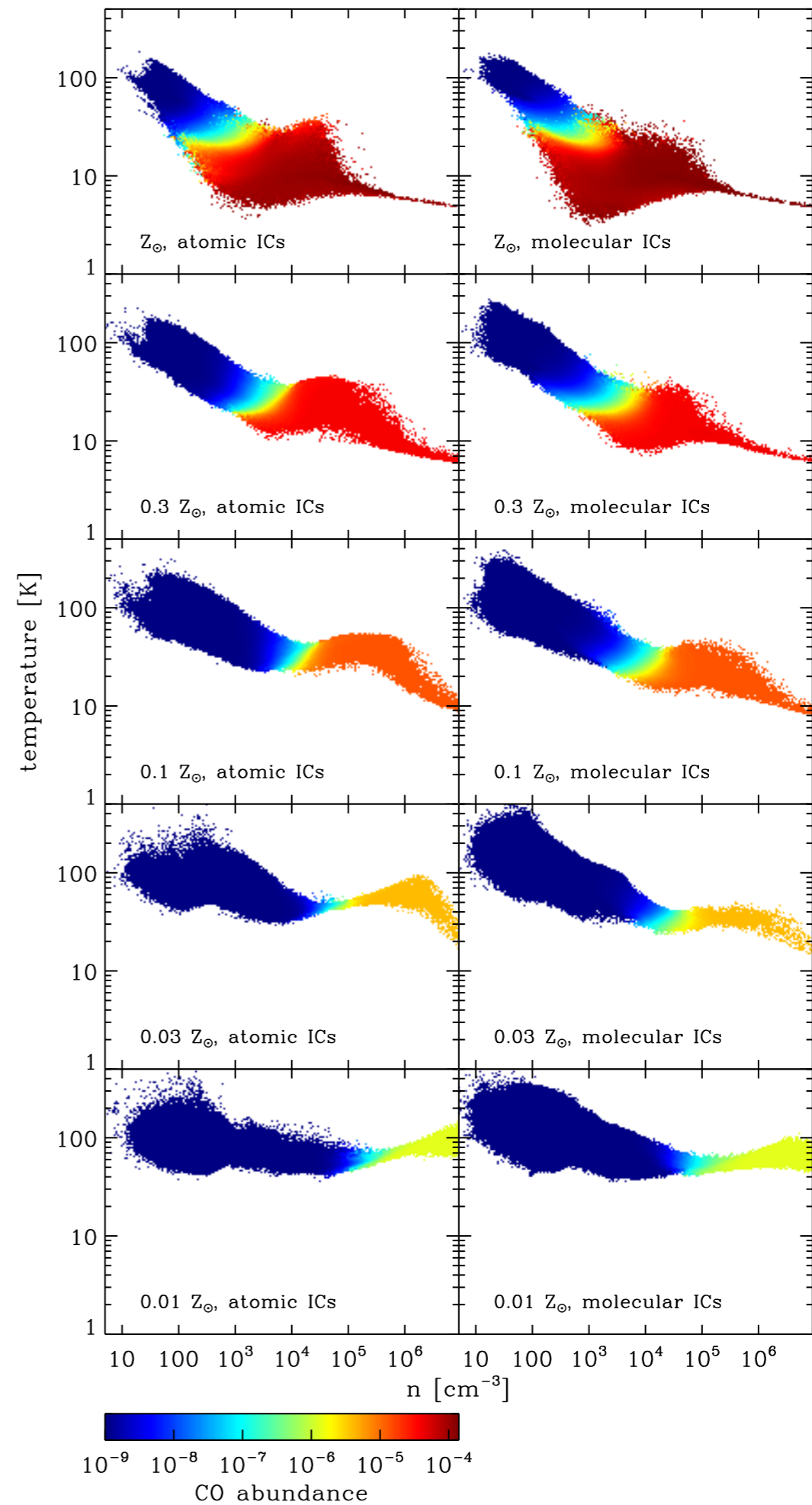
- Can then tabulate the cooling rate for this species in terms of two parameters:
 - T
 - N_X

Science examples

- Can twiddle the parameters of the system to see how star formation changes in different environments.
- In the case on the right, we changed the metallicity in the cloud.
- Star formation rate was not affected
- Chemistry (and observational signatures) is strongly affected.

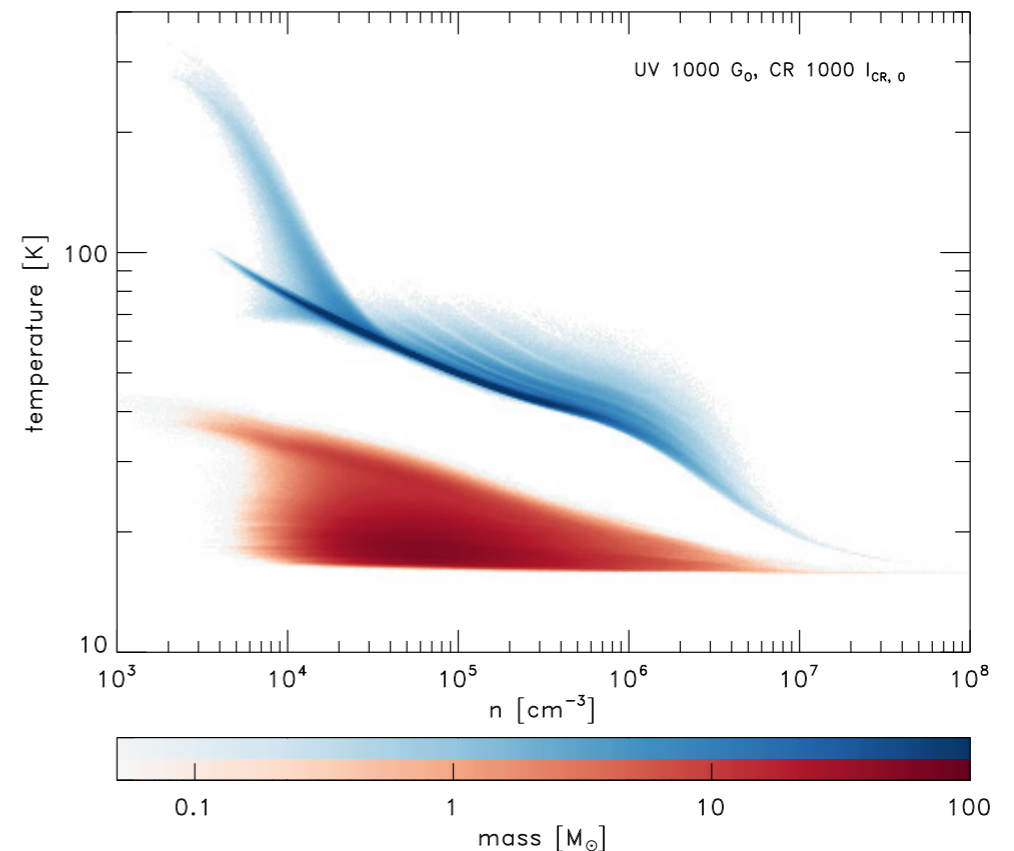
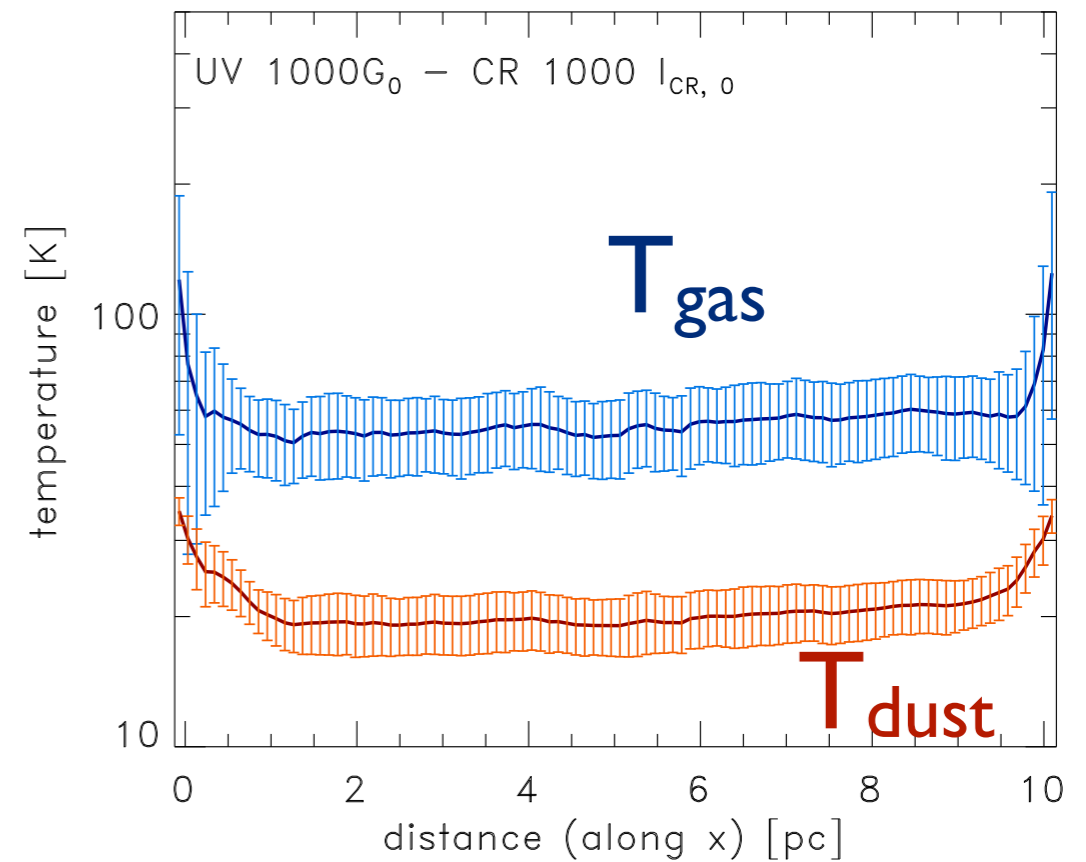


- Metallicity strongly affects the thermodynamics.



Environmental conditions?

- Can also look at changing the strength of the ISRF and the cosmic ray ionisation rate.
- Mimic conditions in the galactic centre.
- To recover the observed gas and dust temperatures, we needed conditions 1000 x more harsh than those in the solar neighbourhood.



Cooling?

- Unlike a standard GMC, clouds in the galactic centre cool via OI line cooling (and then dust).
- Observational prediction.

