Simulating gas dynamics in galaxies: A 3D view of star formation and feedback

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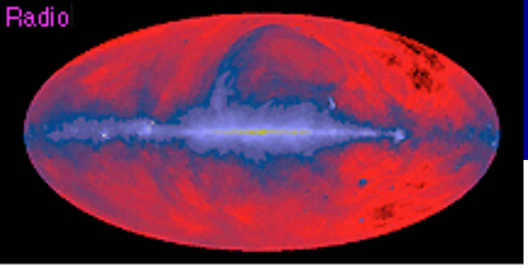
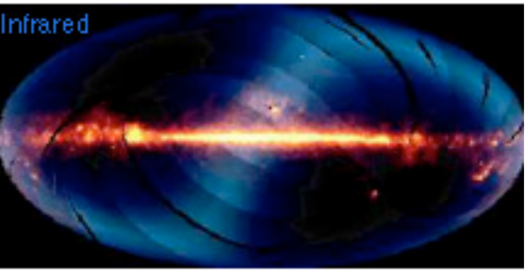
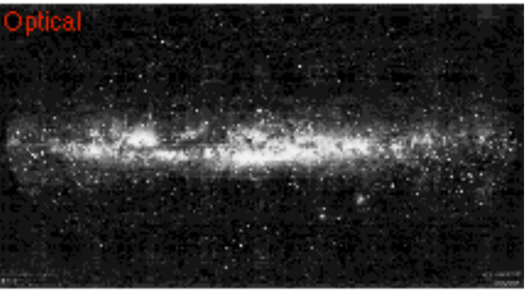
711. WE-Heraeus-Seminar
'The Science Cloud'
Bad Honnef , 15.1.2020

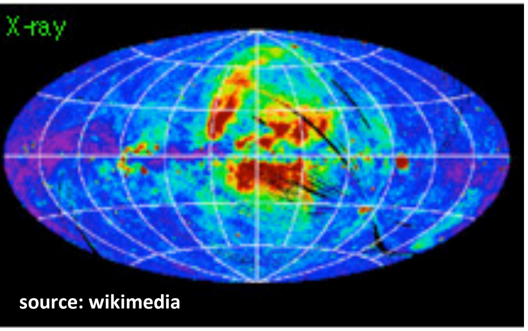
erc
European Research Council
SFB 956
Cologne | Bonn
DFG Priority Program 1573
ISM-SPP
Interstellar Medium
The SILCC project
GCS
Gauss Centre for Supercomputing

Multi-wavelength Milky Way

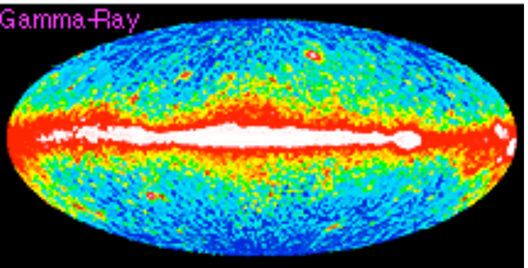




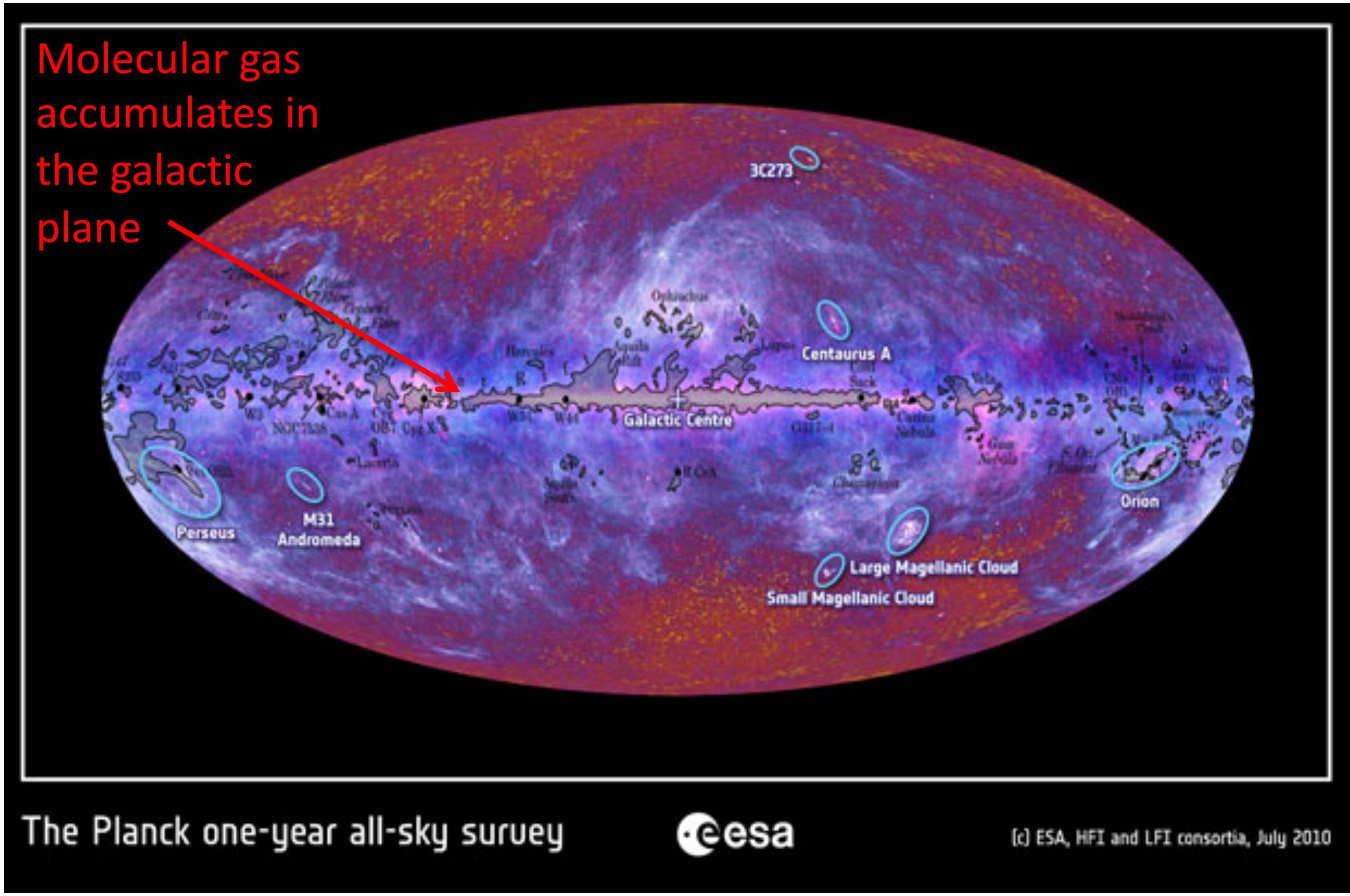




source: wikimedia



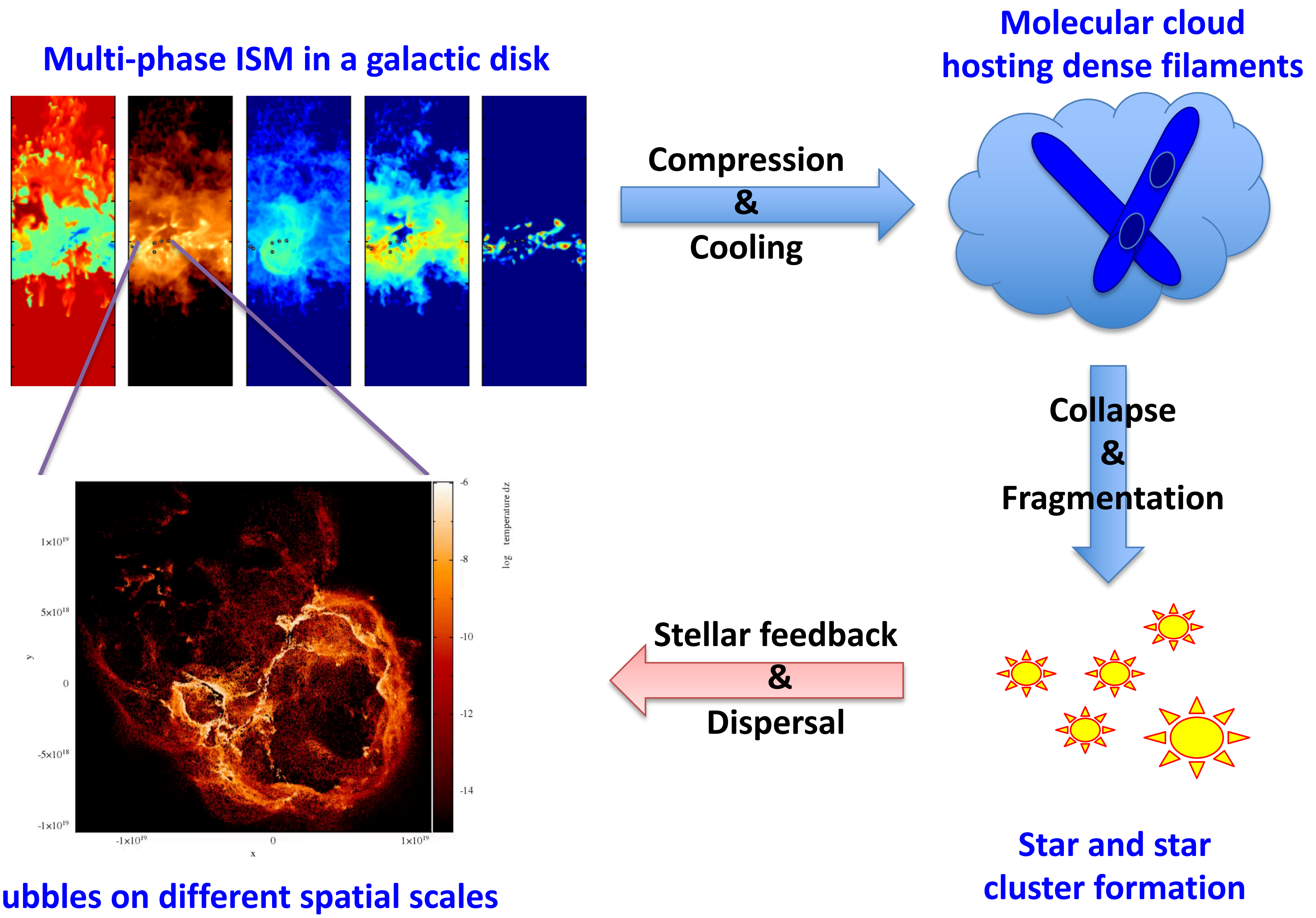
superimposed contours: CO survey (Dame et al. 2001):



Molecular gas accumulates in the galactic plane

Volume filling fractions:
Mihalas & Binney (1981); Kulkarni & Heiles (1988)

The life-cycle of gas in the multi-phase interstellar medium: A schematic view



Multi-phase ISM in a galactic disk

Compression
&
Cooling

Molecular cloud
hosting dense filaments

Collapse
&
Fragmentation

Star and star
cluster formation

Stellar feedback
&
Dispersal

Bubbles on different spatial scales

The conditions of star formation: setting the stage with an example

Orion Nebula within the
Orion A molecular cloud

Nearest massive
star-forming region

Distance ~ 1,350 light years
~ 414 pc (parsec)

Age ~ 3 Myr

Mass ~ 10^5 $M_\odot$

Temp. (dense gas) ~ 10 K

An Orion Nebula Comparison

Spitzer Space Telescope • IRAC

Visible: NOAO/AURA/NSF/A. Block/R. Steinberg

NASA / JPL-Caltech / S.T. Megeath (University of Toledo, Ohio)

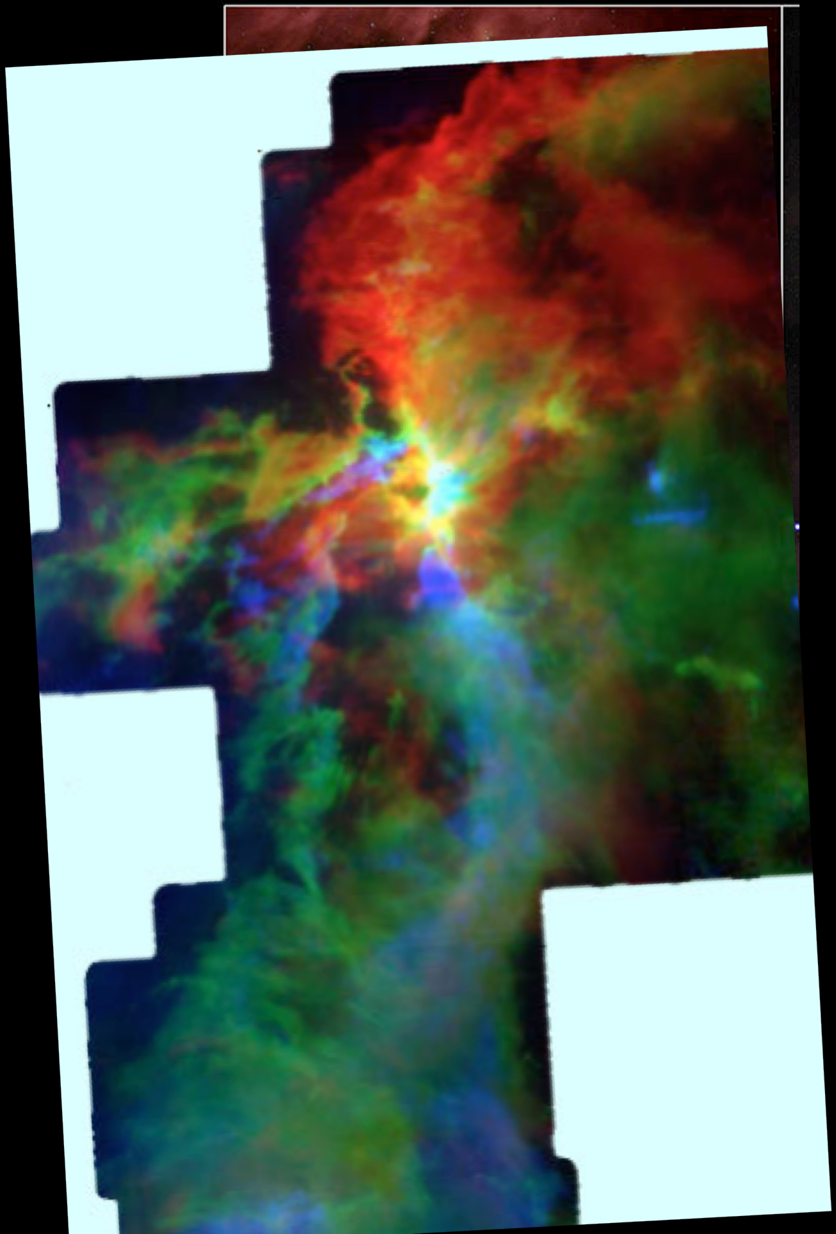
ssc2006-16c

The conditions of star formation: setting the stage with an example

Kong+2018

Carma-Orion survey: velocity-resolved CO

CO forms at a visual extinction of $A_V > 1$ $\Rightarrow$dense gas with column density $\geq 2 \times 10^{21}$ cm^{-2}



velocity range
red: 9.8 -12.1 km/s
green: 7.3 – 9.6 km/s
blue: 4.8 – 7.1 km/s

sound speed @ 10 K ~0.2 km/s

=> Gas in molecular clouds is subject to supersonic turbulence

The conditions of star formation: setting the stage with an example

Friesen +2017

Orange:
NH_3 from the Greenbank Ammonia Survey (GAS)

very dense gas with high visual extinction of A_V>7 (column density ≥1.4 x 10^{22} cm^{-2})

Background:
Blue: Spitzer WISE

Large dynamic range in density within the molecular cloud

dense gas:
10^2 cm^{-3} ≤ n ≤ 10^6 cm^{-3}

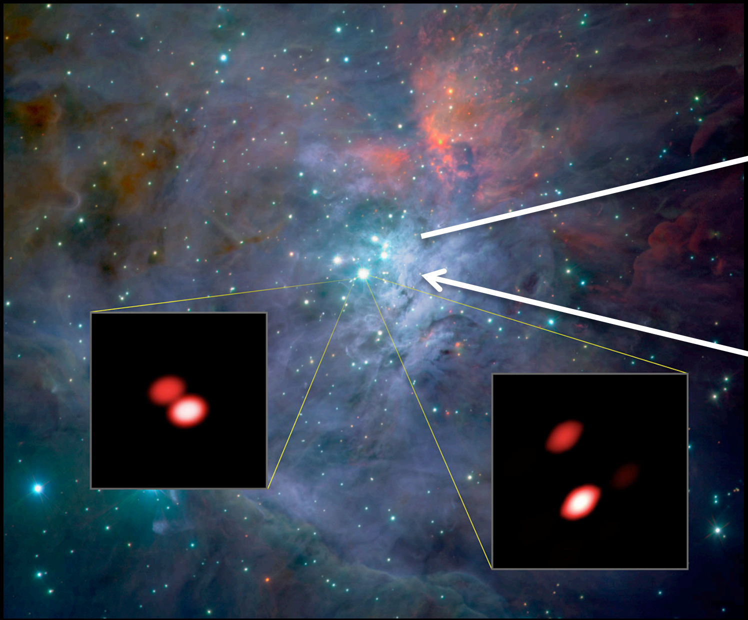
prestellar cores:
n > 10^6 cm^{-3}

The impact of star formation:
Massive star formation and feedback in Orion

Orion Nebula:

Age ~ 3 Myr
Mass ~ 10^5 Msun

Trapezium cluster



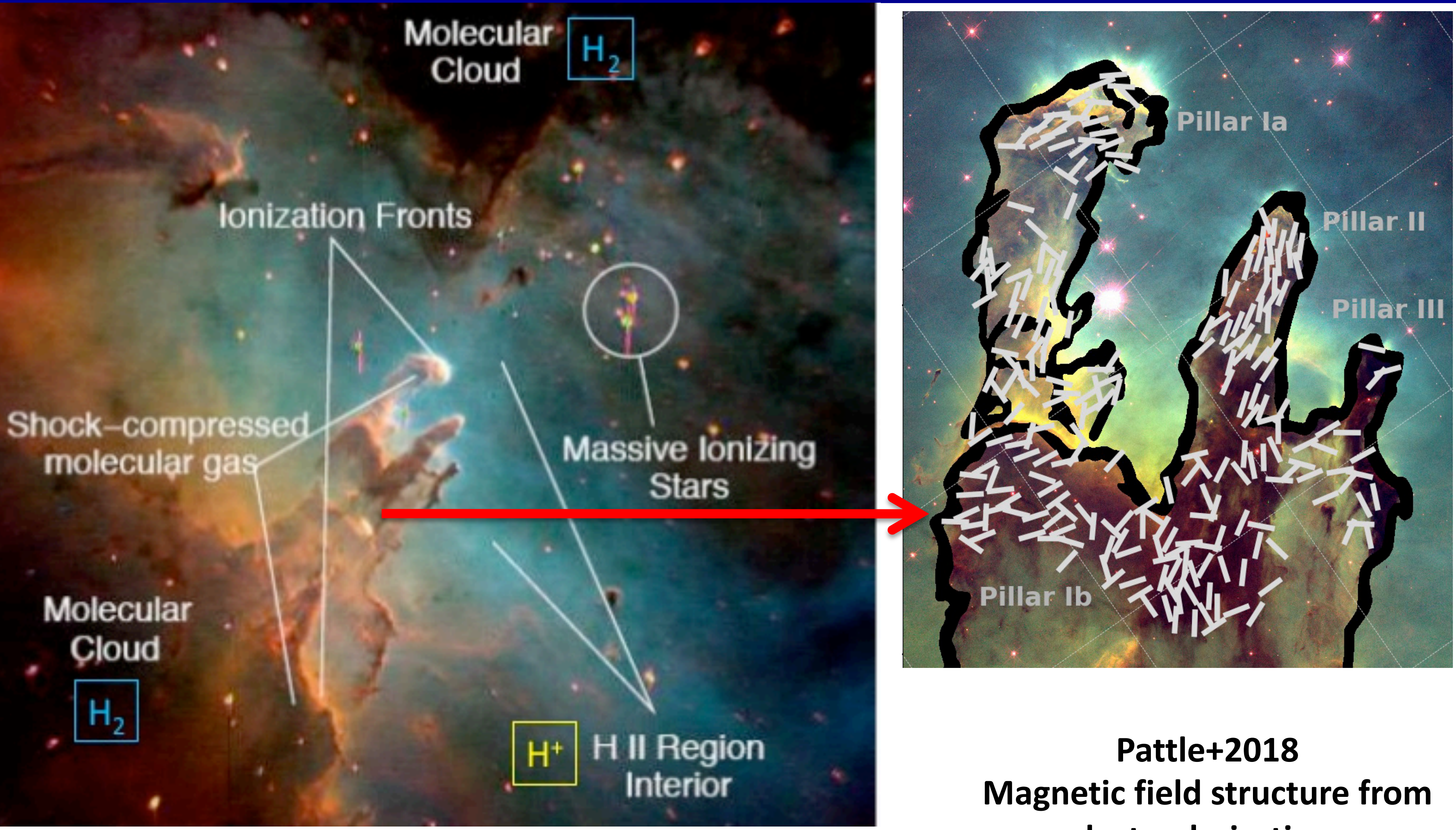
Trapezium Cluster (Orion Nebula)
NASA & K. Luhmann (Harward-Smithonian CfA)
STScI-PRC00-19, WFPC2, NICMOS (Infrared)

Trapezium cluster:

Radius ~ 1.5 light years
~ 0.46 pc
Age ~ few 10^5 years
5 brightest stars: 15-30 $M_\odot$

Binary Theta 1 Orionis F
discovered in 2016 with VLTI-Gravity

The multi-phase interstellar medium: setting the stage with an example



Pattle+2018
Magnetic field structure from dust polarization

Multi-phase interstellar medium

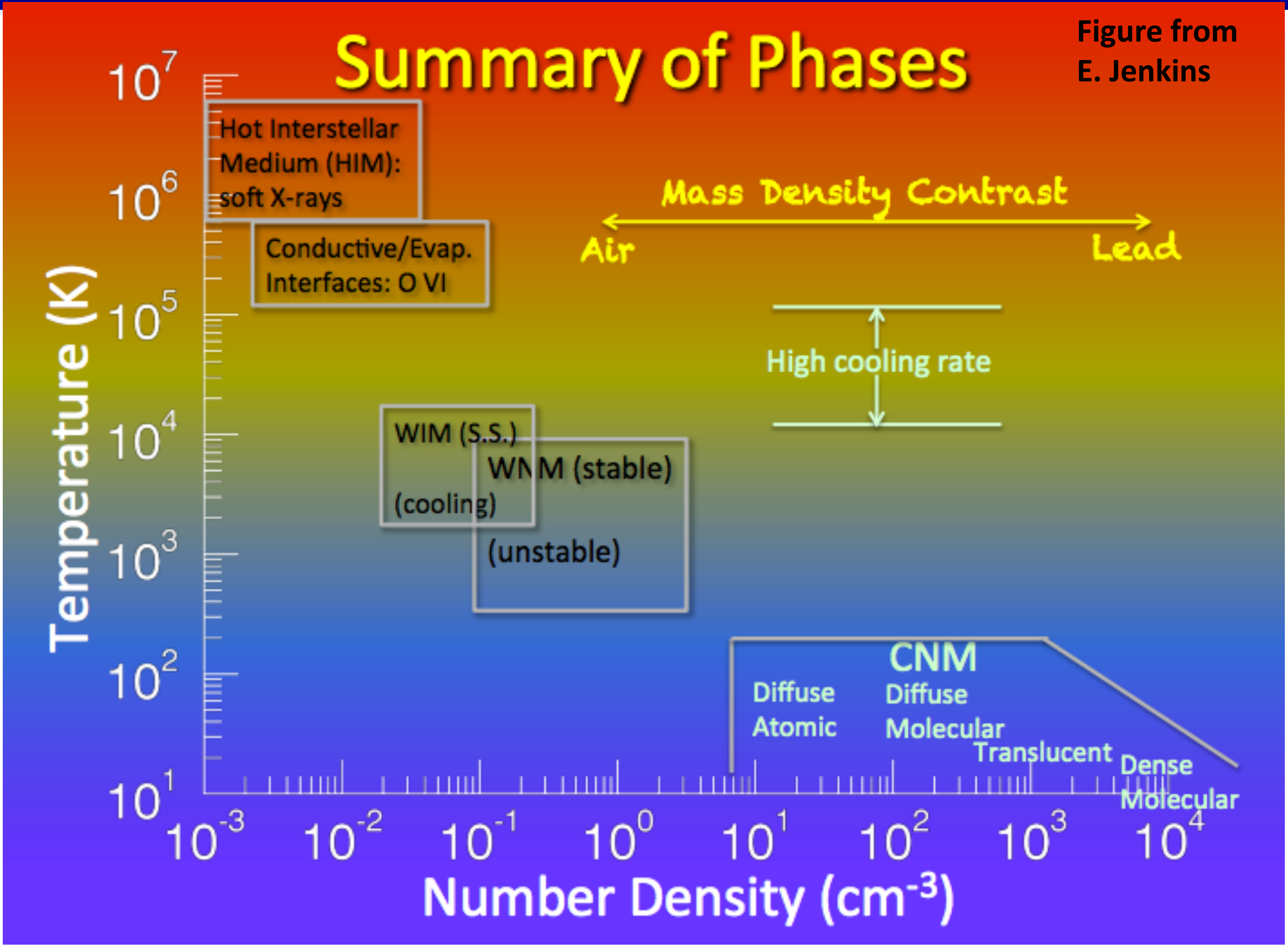


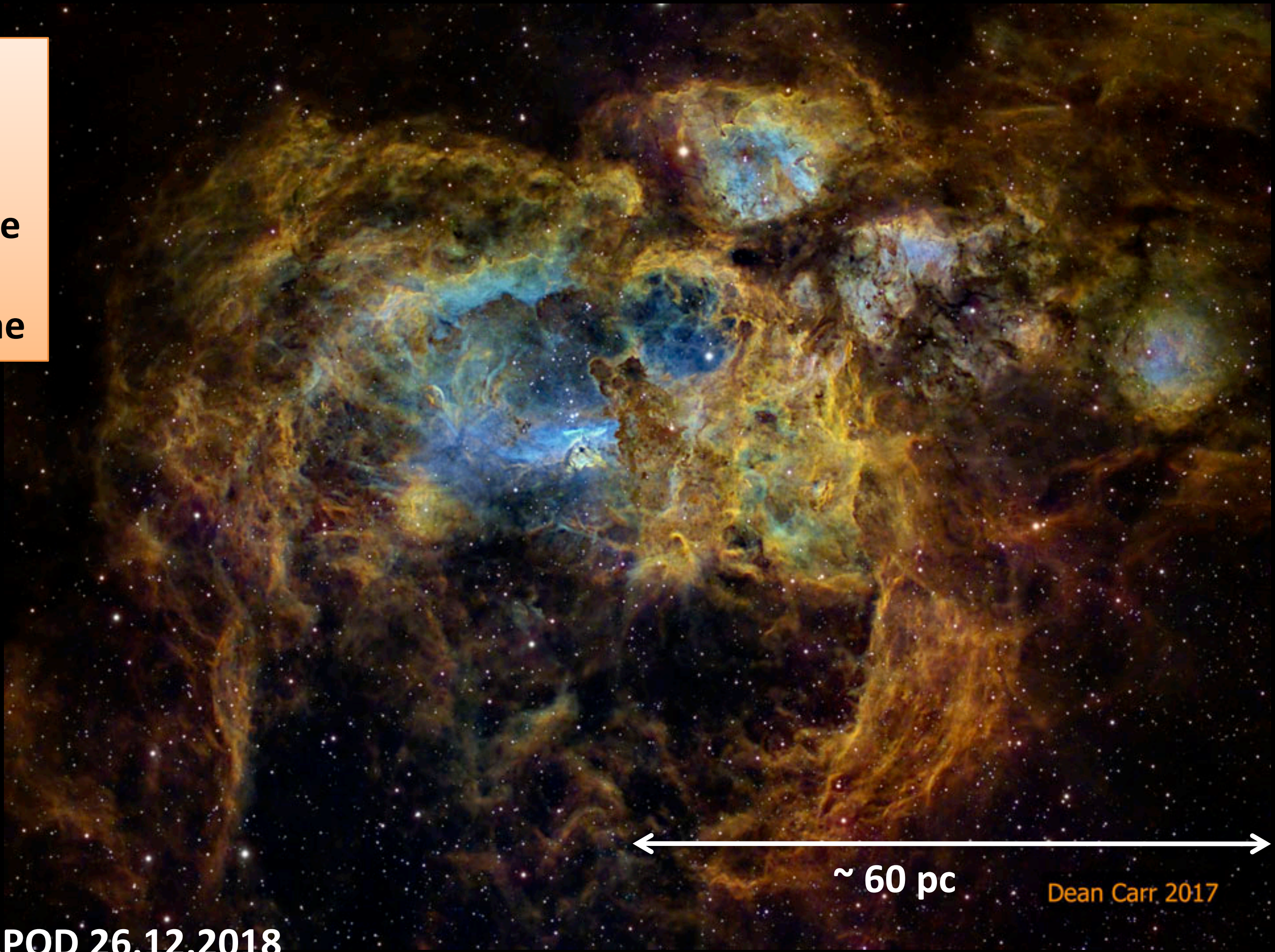
Figure from E. Jenkins

The impact of star formation:
The signatures of stellar feedback are ubiquitous in the ISM

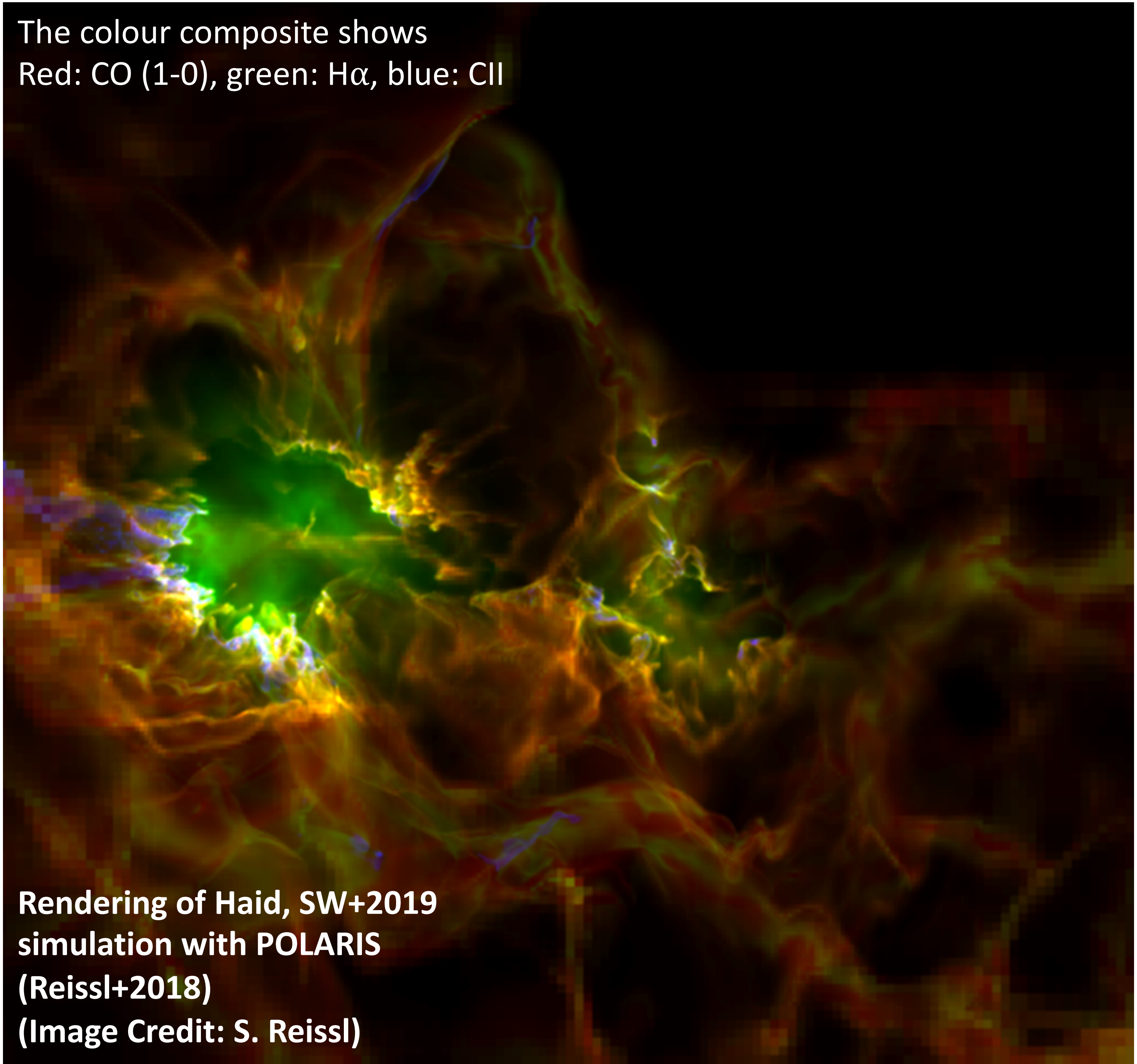
Stellar feedback driven bubbles in the Lobster Nebula (NGC 6357)

Stellar feedback:

- -UV radiation
- -Radiation pressure
- -Stellar winds
- -Type II Supernovae



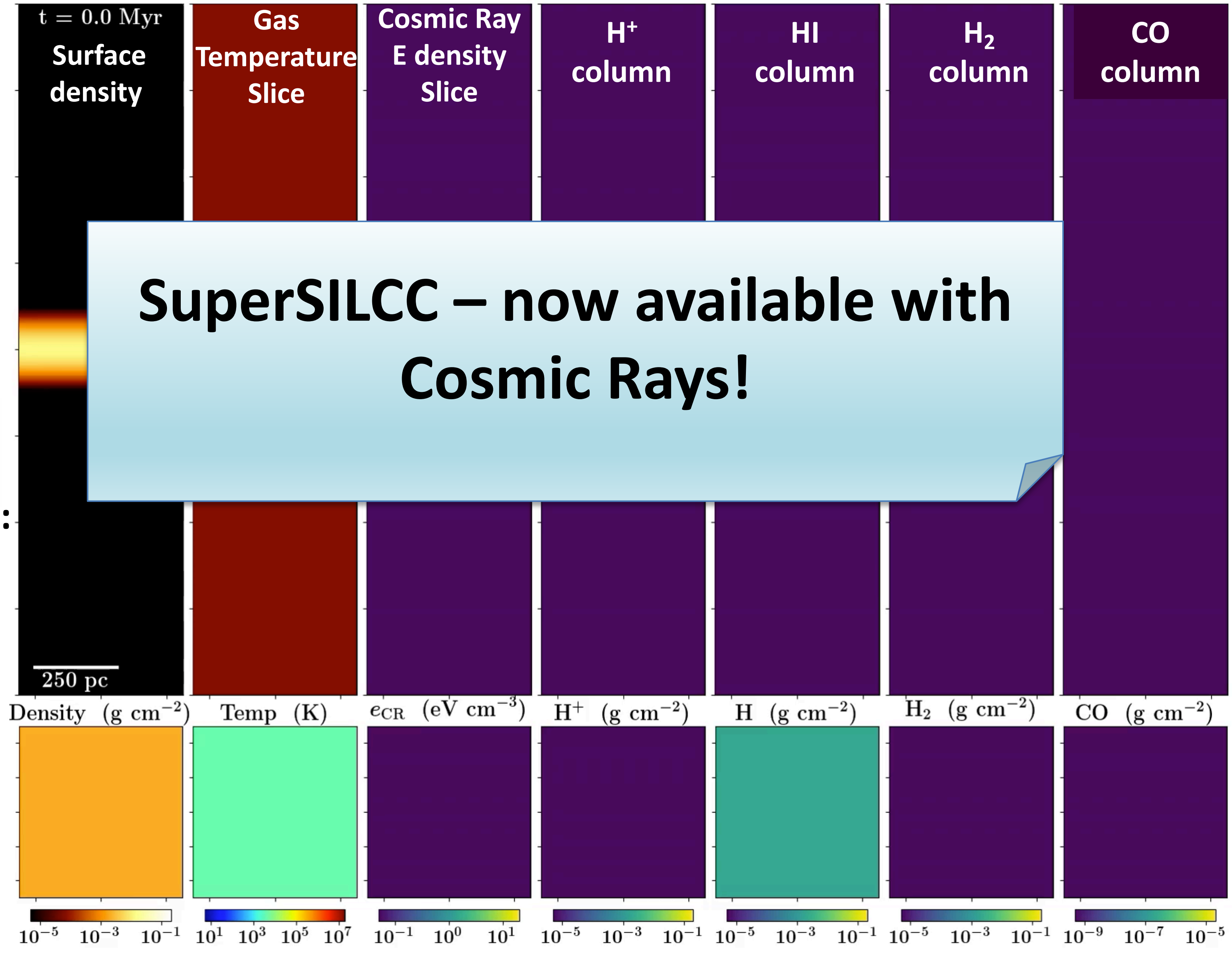
Blue: ionized gas
Red: dust
Image taken from: APOD 26.12.2018



The colour composite shows
Red: CO (1-0), green: Hα, blue: CII

Rendering of Haid, SW+2019
simulation with POLARIS
(Reissl+2018)
(Image Credit: S. Reissl)

New SILCC simulations: SuperSILCC
Stellar winds, Ionizing radiation, Supernovae + Cosmic Rays



SuperSILCC – now available with Cosmic Rays!

Cluster mass:

- $10^2\ M_\odot$
- $10^3\ M_\odot$
- $10^4\ M_\odot$

Walch+2015,
Girichidis+2016,
Gatto+2017,
Girichidis+2018,
Girichidis+in prep.
Dinnbier+in prep.
Rathjen +in prep.

SILCC Project

SImulating the LifeCycle of Molecular Clouds

University of Cologne: S. Walch, D. Seifried, F. Dinnbier, S. Haid
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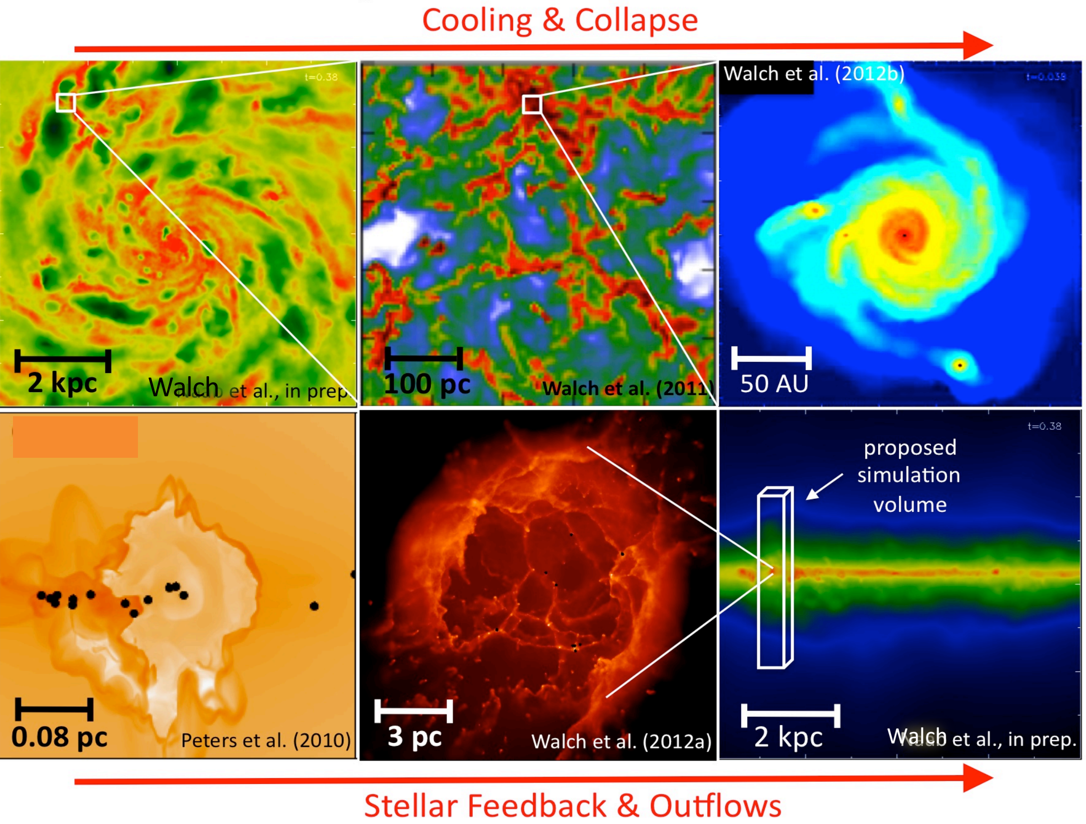
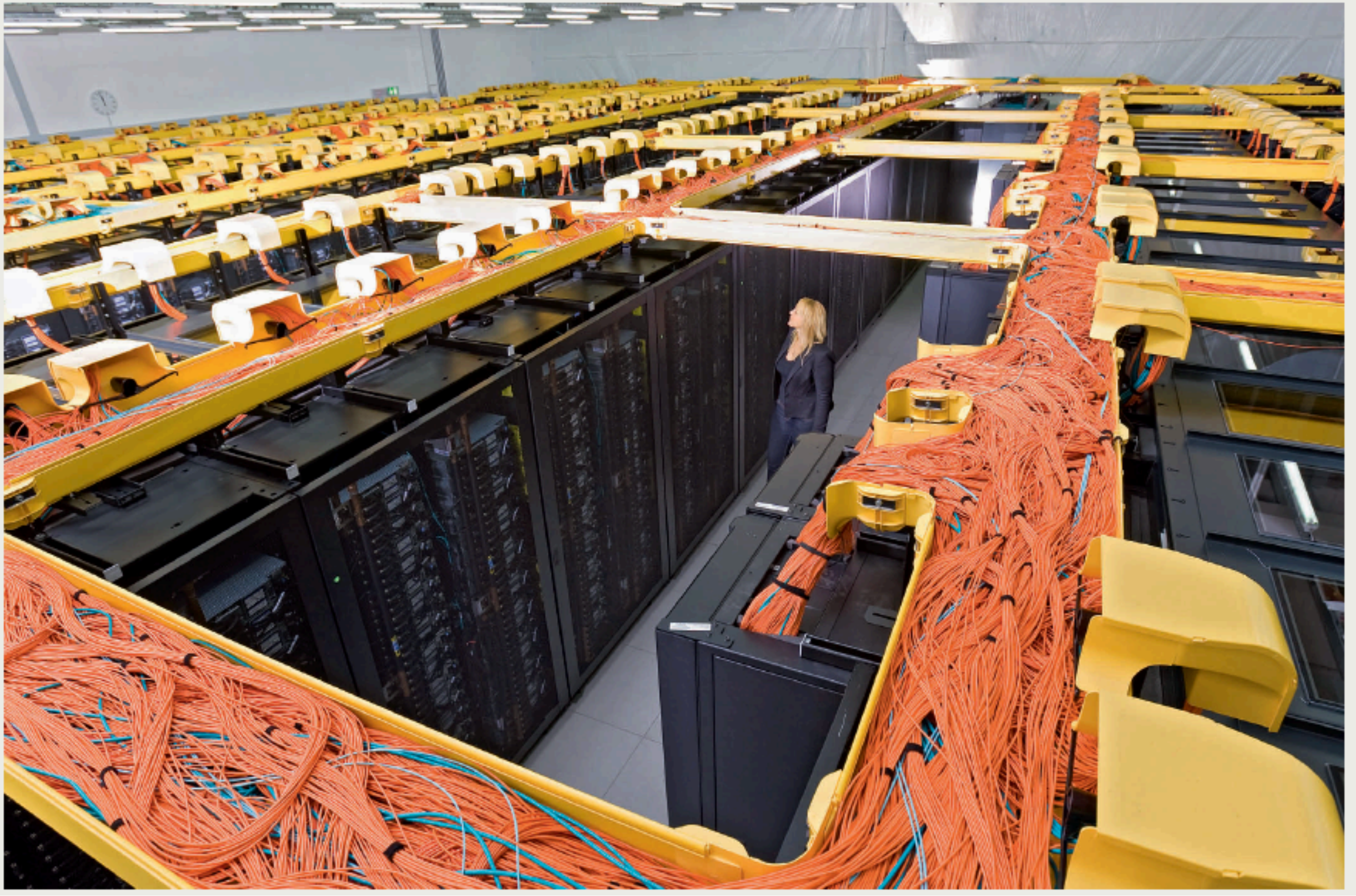


AMR code FLASH 4 with…
- Self-gravity
- External galactic potential
- ideal MHD
- Heating & Cooling and
- Molecule Formation
- TreeRay (diffuse radiation for shielding + radiative transfer from point sources)
- Sink Particles with subgrid cluster model/massive star model
- Supernova Feedback
- Wind
- Cosmic Rays

www.astro.uni-koeln.de/~silcc

Walch +15, Girichidis +16
Peters+17, Gatto+17, Seifried+17, +18

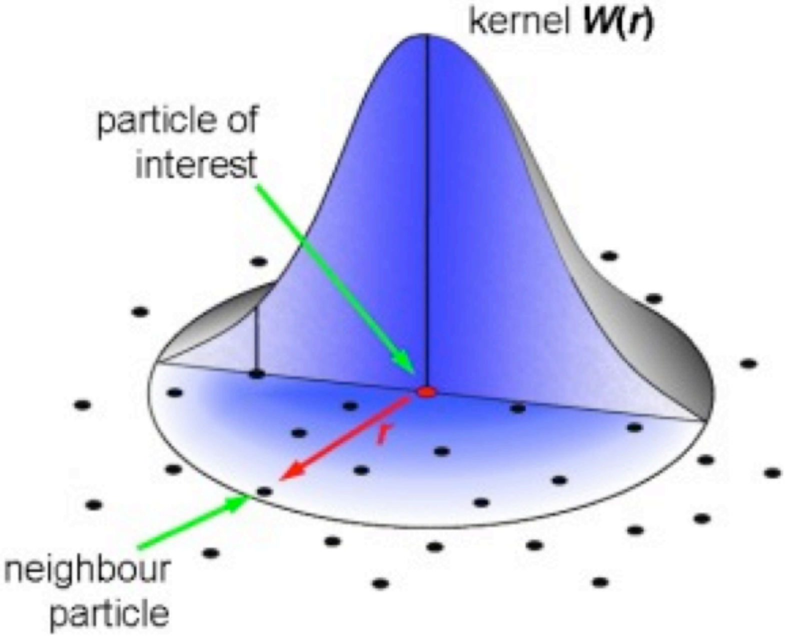
Numerical simulation and high-performance computing: 3 Gauss projects over past 7 years ~150 million core hours on SuperMuc @ Leibniz-Rechenzentrum Garching



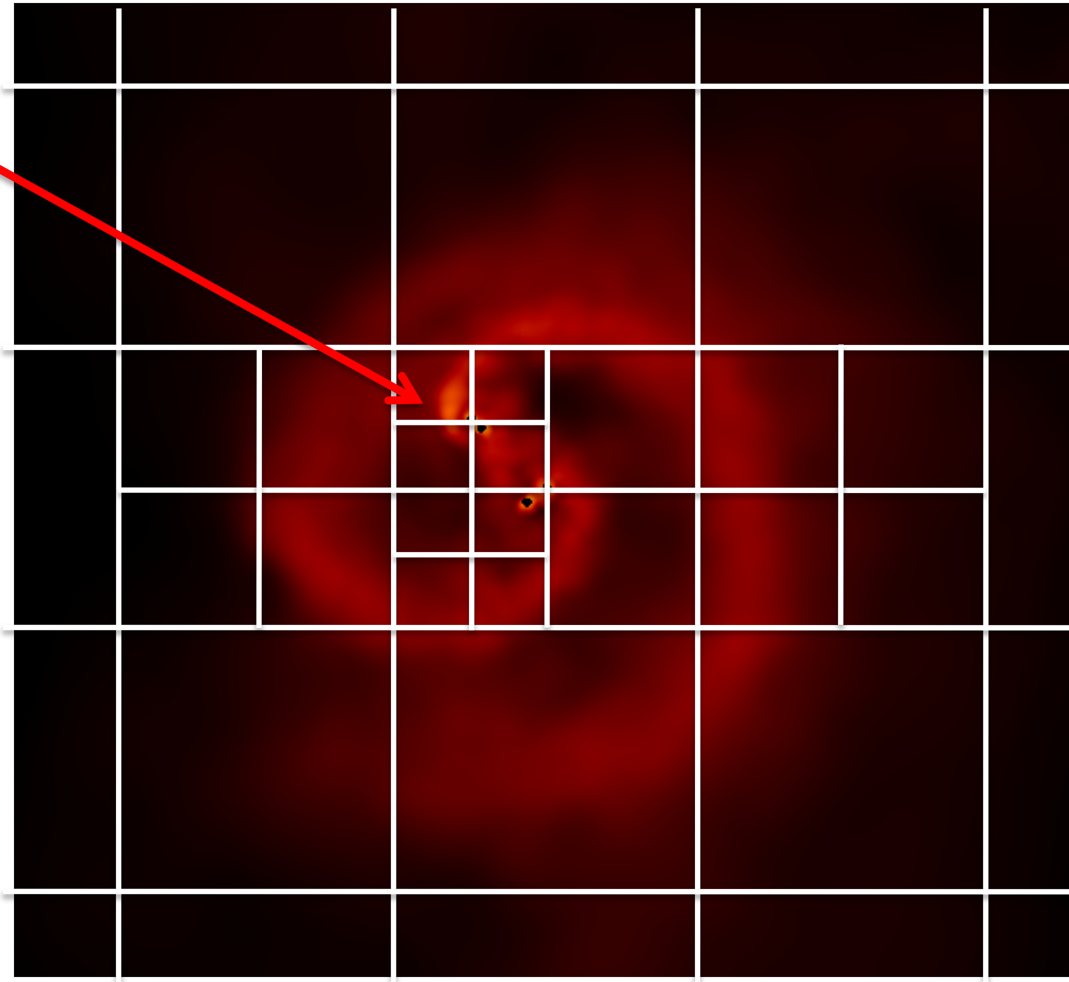
How do we model this?

Lagrangian approach:
Smoothed Particle Hydrodynamics

Fluid quantities in 3D
(In every cell / particle):
Mass or Density ρ
Velocity v_x,v_y,v_z
Temperature or pressure
Ionisation state
Magnetic field, …



Eulerian approach:
Grid-based method with Adaptive Mesh Refinement (AMR)



Let’s have a look at the equations…
(1) Ideal MHD equations + (self-)gravity

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

Conservation of momentum:

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{v} = \frac{(\mathbf{B} \cdot \nabla)\mathbf{B}}{4\pi} - \nabla P_{\text{tot}} + \rho \mathbf{g},$$

Conservation of total energy:

$$\frac{\partial E}{\partial t} + \nabla \cdot \left[(E + P_{\text{tot}}) \mathbf{v} - \frac{(\mathbf{B} \cdot \mathbf{v}) \mathbf{B}}{4\pi} \right] = \rho \mathbf{v} \cdot \mathbf{g},$$

Induction equation:

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B}), \quad \nabla \cdot \mathbf{B} = 0, \longleftarrow$$

Additional constraint from Maxwell: no magnetic monopoles!

where: $E = E_{int} + E_{kin} + E_{mag}$

Closure relation: Ideal gas: $P = (\gamma - 1)\rho\epsilon$

gravitational acceleration : $\mathbf{g}(\mathbf{x}) = -\nabla \phi(\mathbf{x})$

Information travels with the speed of sound / the Alfven speed << speed of light!

$c_{sound} \sim T^{1/2}$

$c_{Alfven} \sim B\, \rho^{-1/2}$

=> Mach number, Alfvenic Mach number

Chemical evolution: Multispecies

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{v}) = C_i(\rho, T, \ldots) - D_i(\rho, T, \ldots)$$

(Self-)Gravity

Solve the Poisson equation:
relating density and
gravitational potential

$$\nabla^2\phi(\mathbf{x}) = 4\pi G\rho(\mathbf{x})$$

Can be gas + stars + dark matter

Gravity is a long-range force!
The exact solution requires solving an N^2 problem.

Solution using the **Green's function**: $$\nabla^2 u(\mathbf{x}) = f(\mathbf{x})$$

Laplacian is linear operator => $$u(\mathbf{x}) = \int_{\mathbf{x}'} d\mathbf{x}' G(\mathbf{x},\mathbf{x}') f(\mathbf{x}')$$

with response of system at x
to point source at x' :
(where δ is the Dirac delta function)

$$\nabla^2 G(\mathbf{x},\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}')$$

Solution: **Newtonian potential**: $$G(\mathbf{x},\mathbf{x}') = -\frac{1}{4\pi}\cdot\frac{1}{|\mathbf{x}-\mathbf{x}'|}$$

(Self-)Gravity

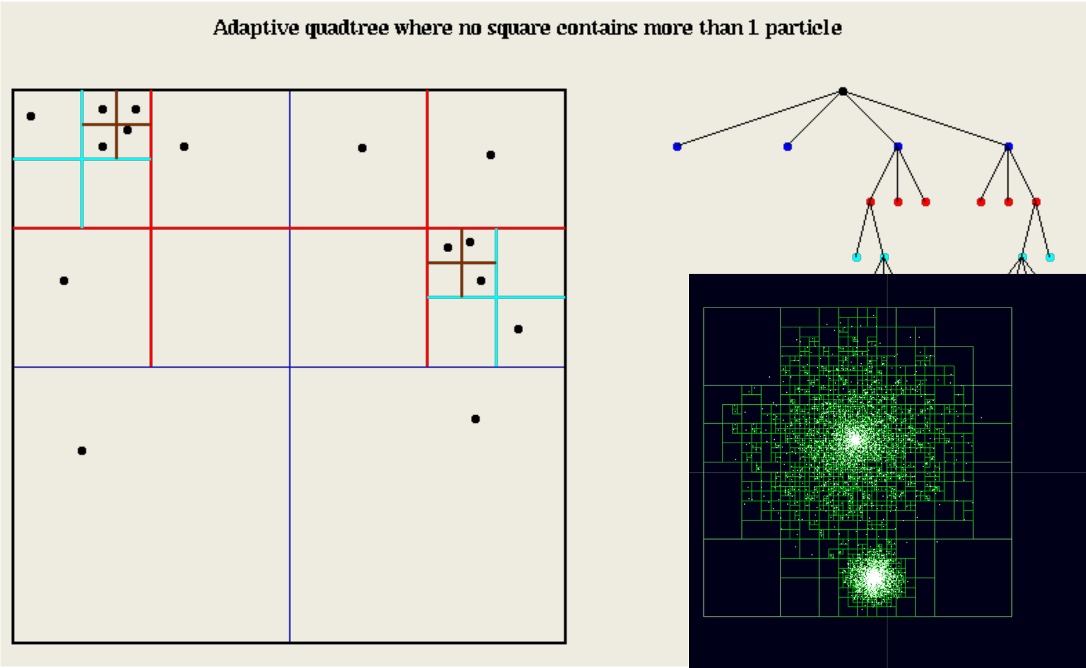
Solve the Poisson equation:
relating density and
gravitational potential

$$\nabla^2\phi(\mathbf{x}) = 4\pi G\rho(\mathbf{x})$$

Gravity is a long-range force!
The exact solution requires solving an N^2 problem.

FLASH implements a multigrid method using V-Cycles

Tree-structure most efficient,
e.g. Octal-spatial tree
(Barnes & Hut 1986)
for neighbor search and
short/long-range
gravitational forces



Diffuse radiation for molecule formation

- Molecules can shield themselves against the interstellar radiation field!
- This process requires radiative transfer of diffuse radiation

- Start with the full RT equation:

$$\frac{\partial I_\nu}{\partial s} = \xcancel{\eta_\nu} - \chi_\nu I_\nu$$

ν = frequency of the photon package

η_ν = emissivity

χ_ν = opacity

I_ν = specific intensity

s= path length along the ray

- We neglect reemission:

$$I_\nu = I_{\nu,0} e^{-\tau_\nu} + \xcancel{\int_0^{\tau_\nu} S_\nu e^{-\tau'_\nu} d\tau'_\nu},$$

S_ν = source function

τ_ν = optical depth

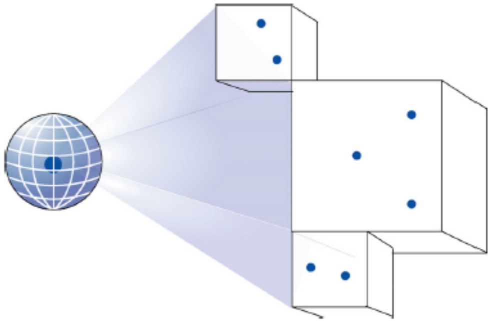
We neglect 2nd term; this is ok if $S_\nu << I_{\nu,0}$ and optical depth τ_ν is not too large.

=> Need to determine τ_ν along a large number of rays, i.e. determine column density of absorber along the rays

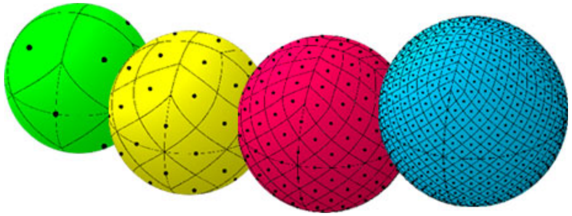
TreeCol

Clark, Glover & Klessen(2012)

FLASH implementation: Wünsch +2018



- **Implementation based on an improved version of the Barnes-Hut tree written by R. Wünsch (FLASH 4.3 release)**
- **Large number of rays still too expensive**
- **Make use of fact that each tree node stores information necessary for computing column densities**
- **Span a HealPix sphere from each cell**
- **During tree-walk to compute gravitational forces: map projected column density of tree-nodes onto this sphere**

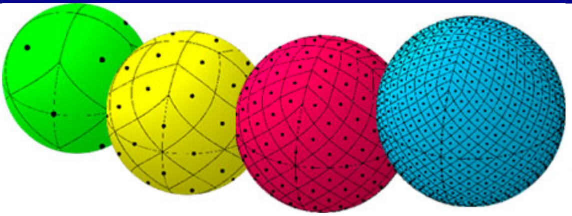


- **To compute the projected column density we need**
  - **the mass of the node**
  - **the node position with respect to the current cell**
  - **the size of the node**
- **We compute:**
  - **total column density -> total Av**
  - **total H_2 and CO column -> self-shielding**
  - **dust attenuation**

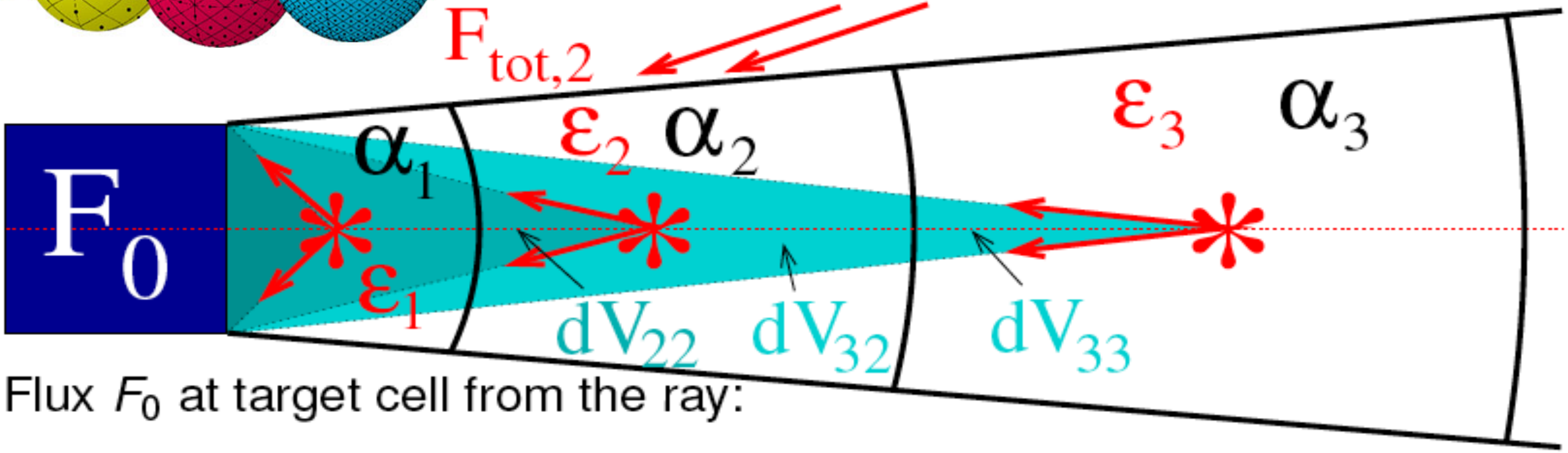
$$\chi(N_{\mathrm{H}}) = \frac{4\pi \int_0^\infty J_\nu \kappa_\nu \exp(-\kappa_\nu \Sigma)\, \mathrm{d}\nu}{4\pi \int_0^\infty J_\nu \kappa_\nu\, \mathrm{d}\nu},$$

TreeRay:
New radiative transfer algorithm
Wünsch, SW, in prep.

European Research Council



Healpix tesselation:
Looking into different directions from each cell

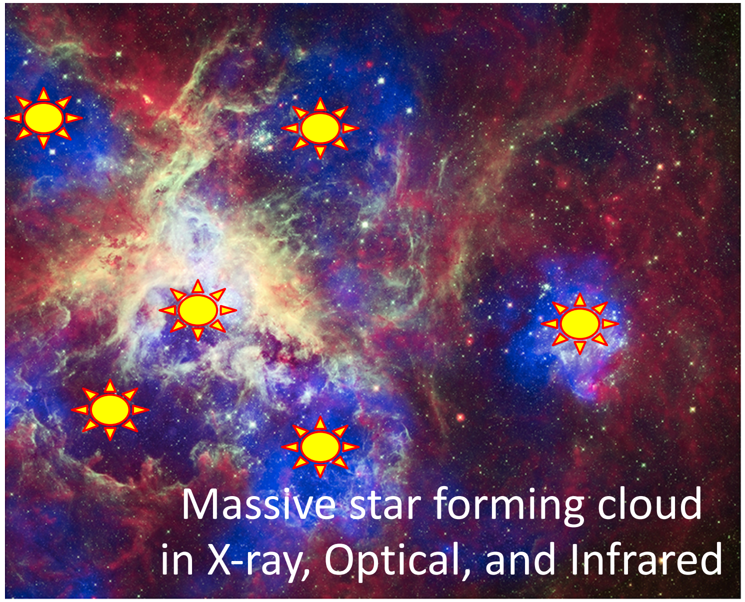


Flux F_0 at target cell from the ray:

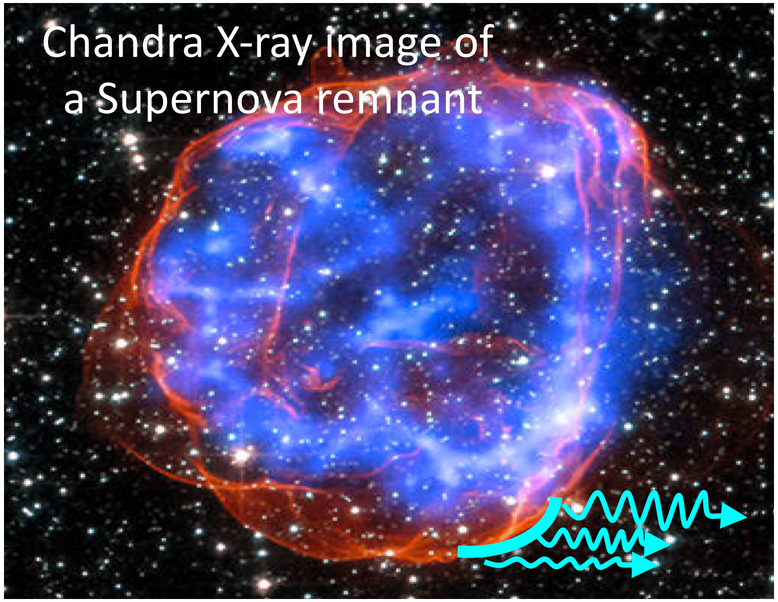
$$F_0 = \sum_{i=N-1}^{0}\left[\frac{\varepsilon_i}{4\pi r_i^2} - \sum_{j=i+1}^{N}\underbrace{\alpha_j F_{ij}}_{\alpha_\star\rho^2/m^2}\frac{F_{ij}}{F_{\text{tot},i}}\mathrm{d}V_{ij}\right]$$

where F_{ij} is flux from source j at segment i and
$\mathrm{d}V_{ij} = \frac{1}{3}\sum[(r_j - r_i)^3 - (r_j - r_{i+1})^3]\mathrm{d}\Omega$
absorption $\sim F_{ij}/F_{\text{tot},i}$ where $F_{\text{tot},i}$ is total flux coming from all rays intersecting with segment $i \rightarrow$ iterations needed

Strengths of TreeRay



Massive star forming cloud
in X-ray, Optical, and Infrared



Chandra X-ray image of
a Supernova remnant

**Multiple point sources
can be treated at very little
extra cost**

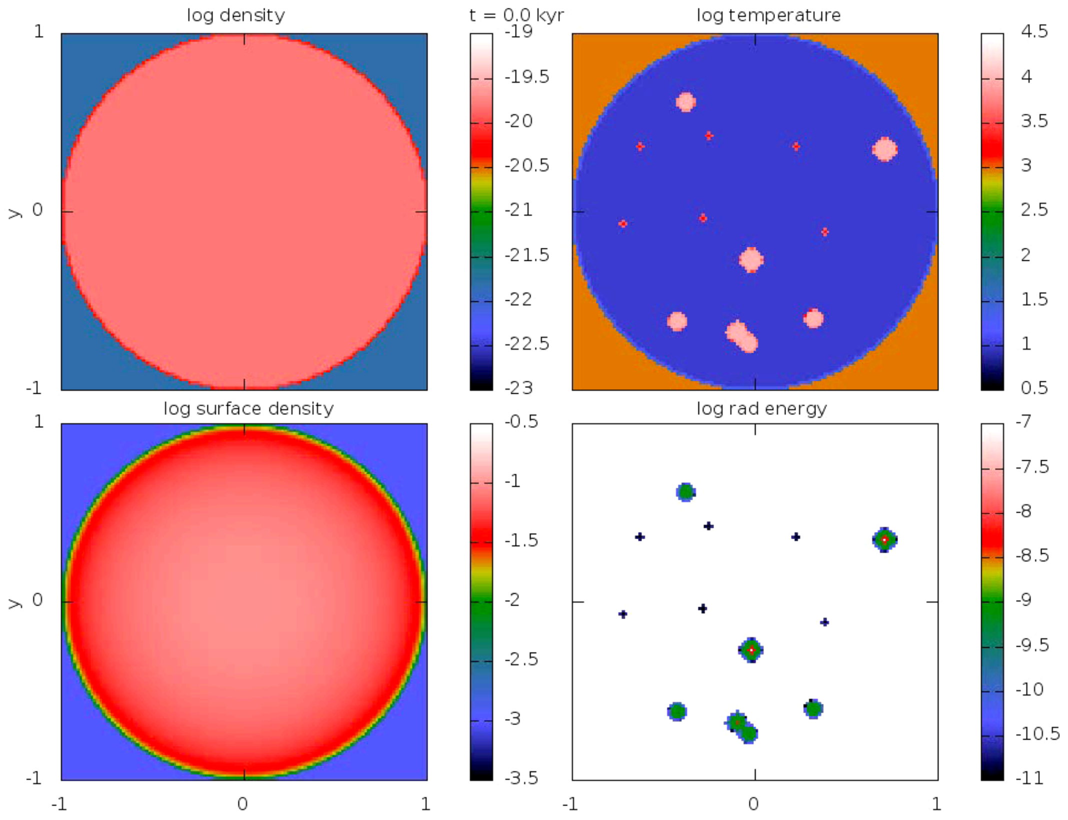
**Re-processing of emission from
radiatively cooling,
high Mach number
shock fronts can be treated!**

TreeRay test:
100 massive stars ionize a molecular cloud

European Research Council

- ★Treat many 100 sources of radiation (every cell can be a source)
- ★ VERY SMALL computational cost if gravity is included!
- ★First successful applications in large-scale 3D simulations

TreeRay allows us to simulate star cluster formation with thousands of radiative sources!



Density slice

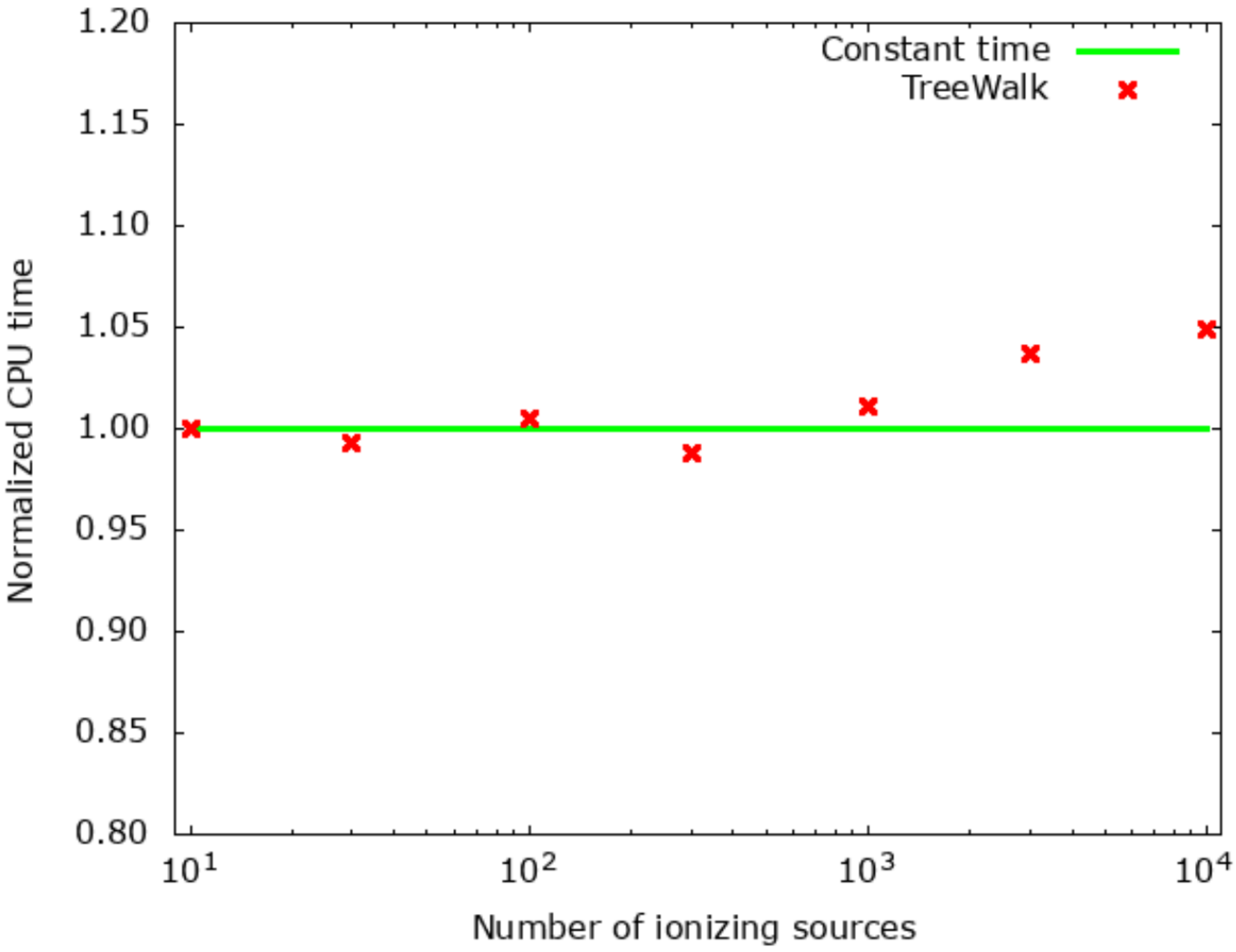
Temperature slice

Surface density

Radiative energy

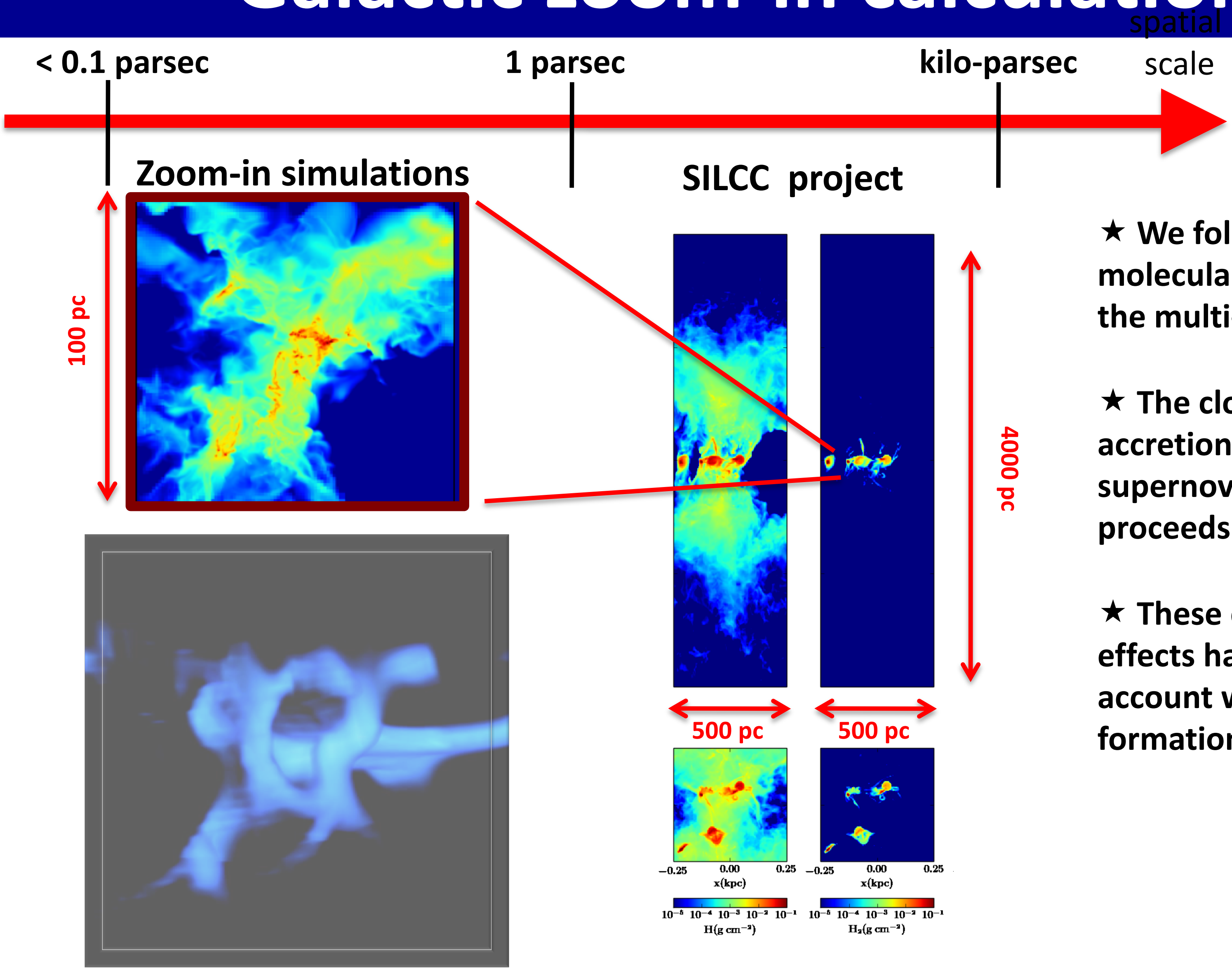
Proof-of-concept published by Walch & Wünsch in the Starbench II code comparison project (Bisbas et al. 2015)

Scaling of TreeRay with # sources



(Wünsch , Walch et al., in prep.)

SILCC-ZOOM: Galactic zoom-in calculations:



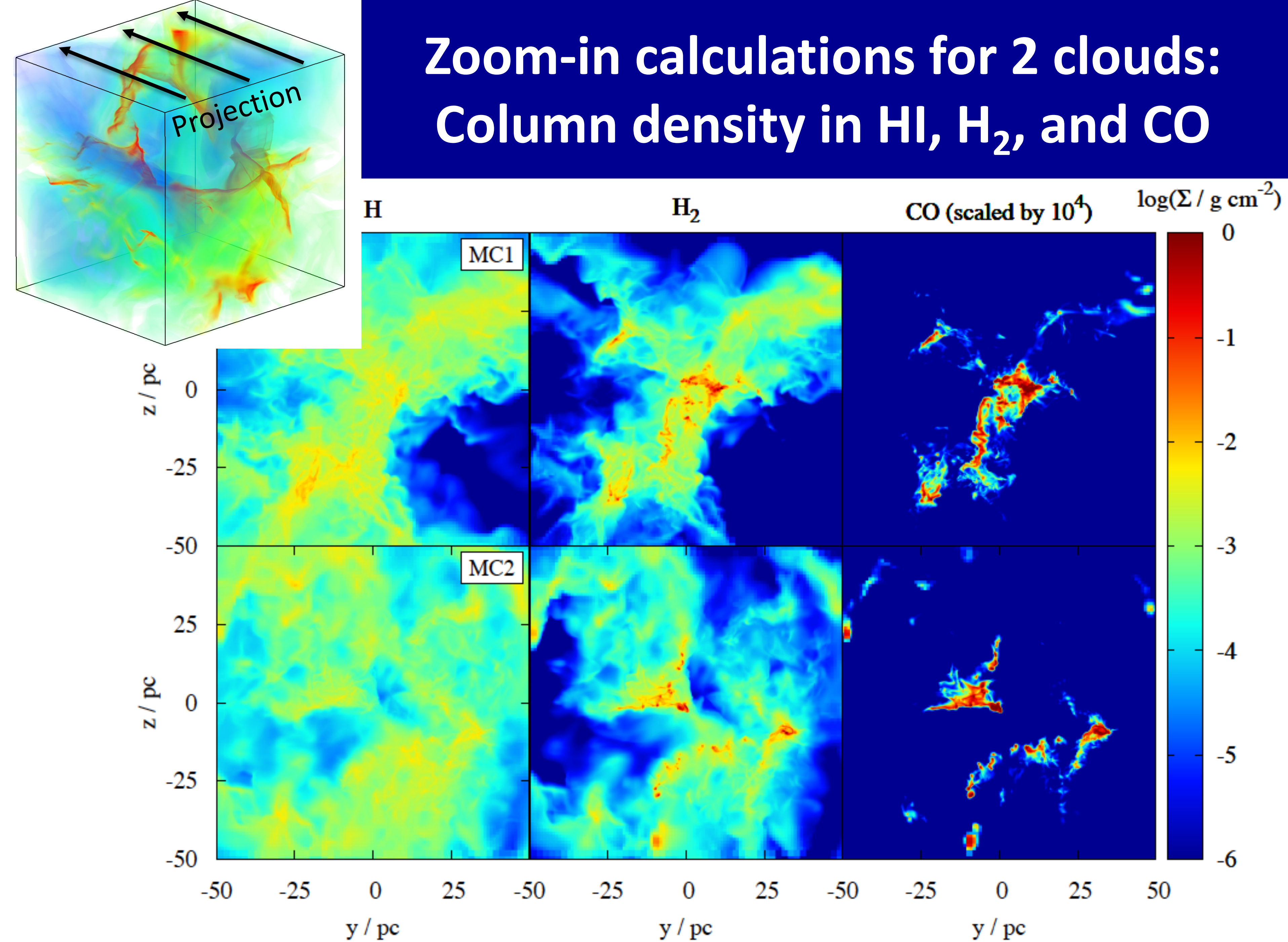
★ We follow individual molecular clouds formed in the multi-phase ISM.

★ The clouds are affected by accretion/merging/nearby supernovae as star formation proceeds.

★ These environmental effects have to be taken into account when studying star formation.

Seifried, SW +2017
Seifried, SW +2018

Zoom-in calculations for 2 clouds: Column density in HI, H_2, and CO



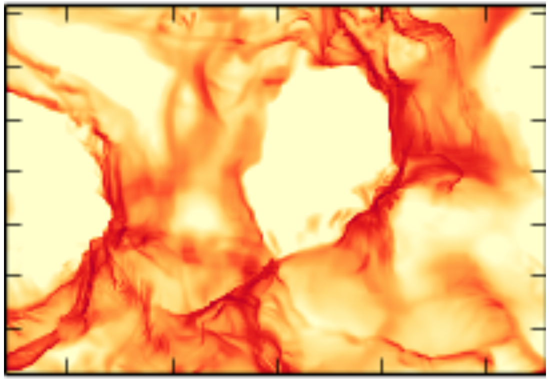
Seifried, SW+2017; includes chemical network Glover+2010; shielding: TreeCol (Clarke+2012; Wünsch, SW+2018)

Comparison of simulations and observations

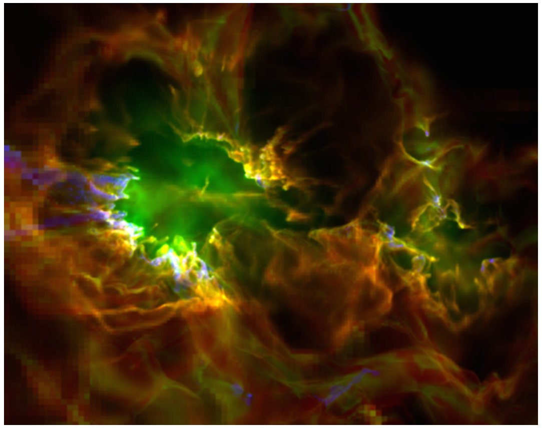
- ★Requires post-processing of the data with radiative transfer tools i.e. RADMC-3D, POLARIS, CLOUDY, MAPPINGS-V

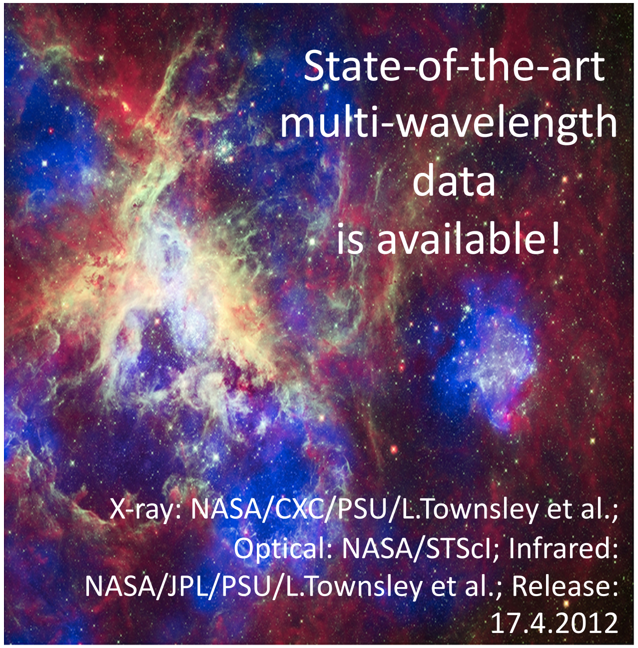
- ★Pipeline for FLASH-to-RADMC-3D available

CII line emission study Franeck +2019 with RADMC-3D
PhD thesis of A. Franeck 10/2018



Rendering of Haid+18b simulation with POLARIS (Image Credit: S. Reissl)





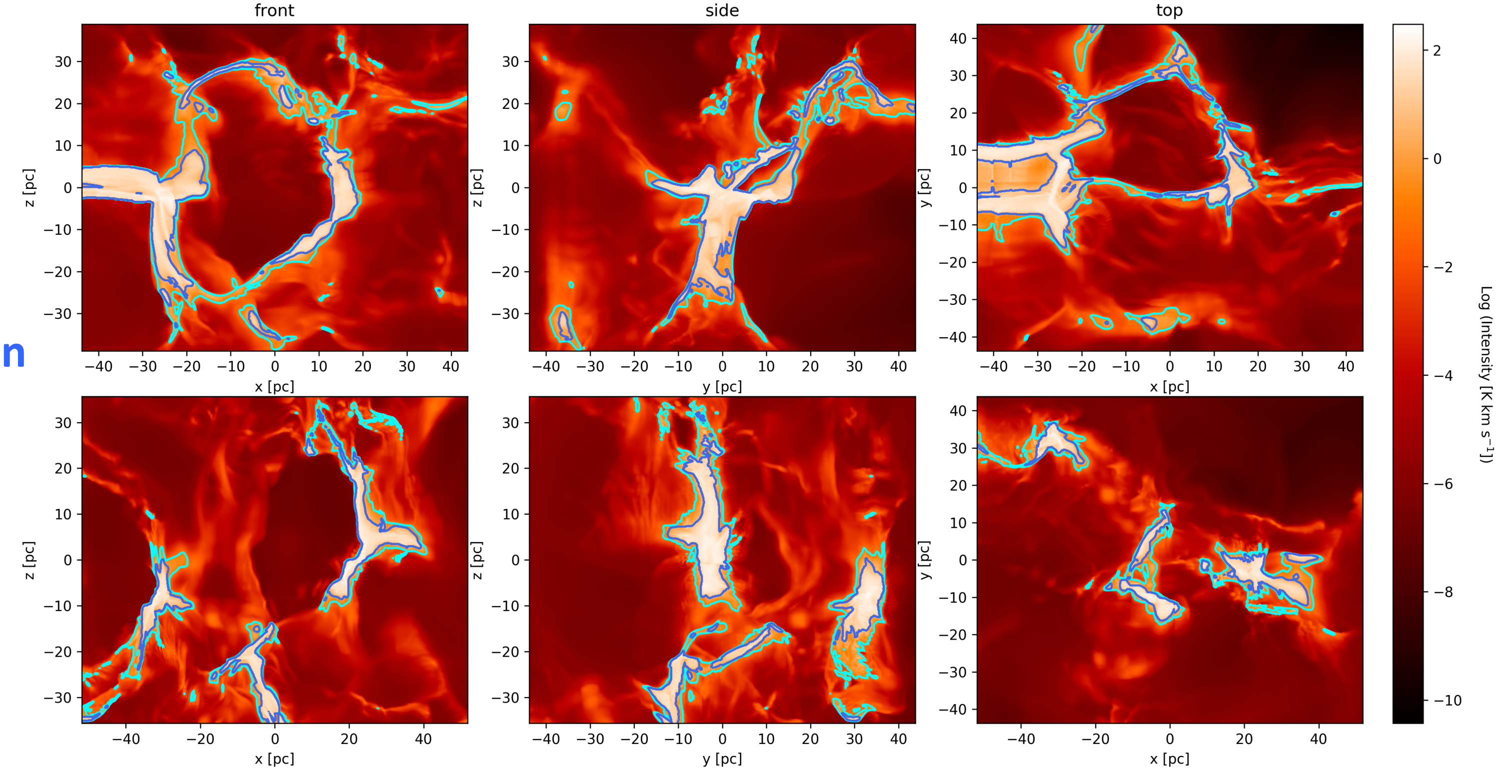
State-of-the-art multi-wavelength data is available!

X-ray: NASA/CXC/PSU/L.Townsley et al.; Optical: NASA/STScI; Infrared: NASA/JPL/PSU/L.Townsley et al.; Release: 17.4.2012

Synthetic CO emission maps for 3D molecular clouds

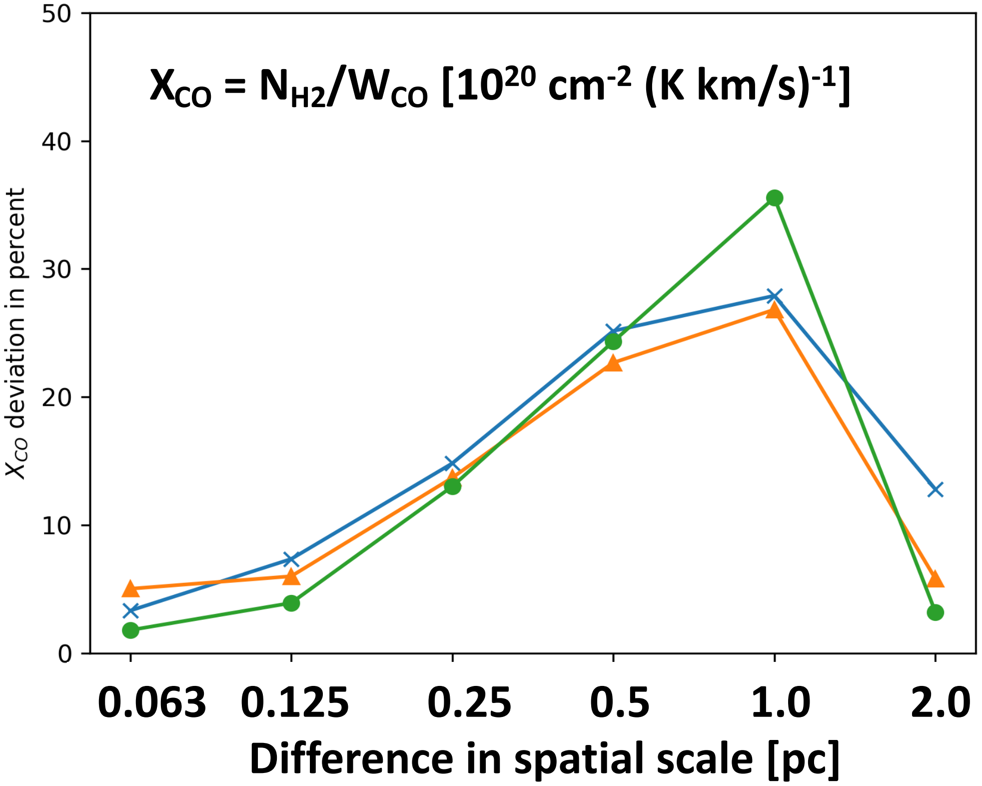
MC1
different LOS
green:
observable area
blue:
optically thick region

MC2
different LOS

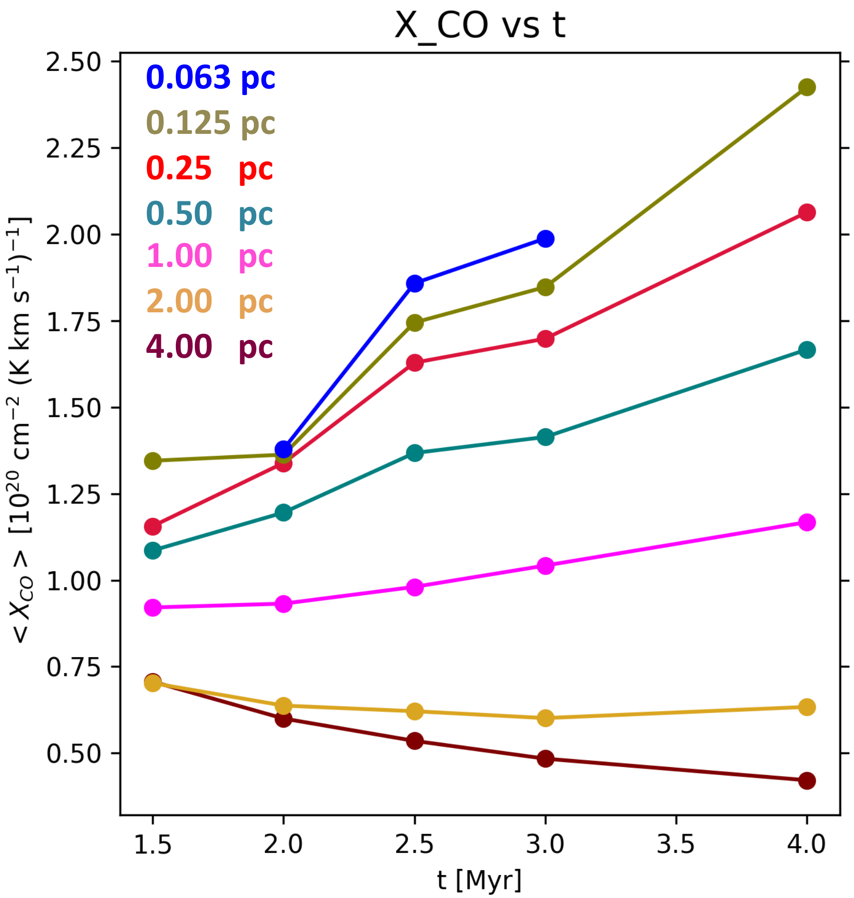


Master thesis of E. Borchert, Borchert et al., in prep.

Synthetic CO emission maps for 3D molecular clouds



$X_{CO} = N_{H2}/W_{CO}$ [10^{20} cm^{-2} (K km/s)$^{-1}$]



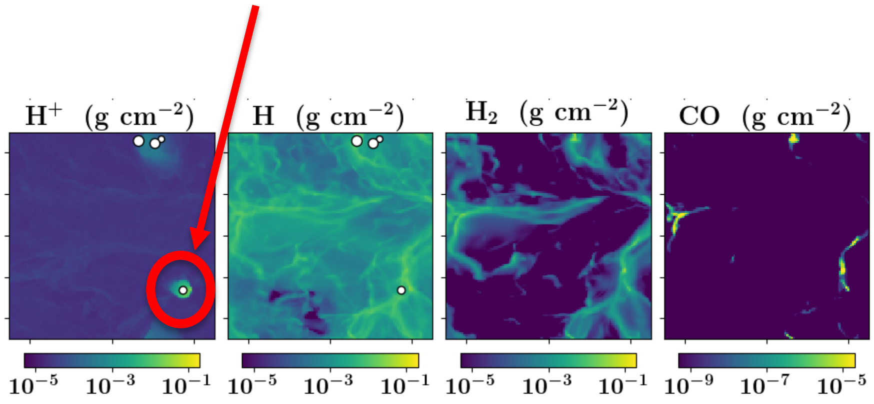
Sub-parsec resolution required to converge in X_{CO}

Time evolution of X_{CO}:
Increase in X_{CO} as the cloud is formed,
as long as the resolution is high enough to resolve it

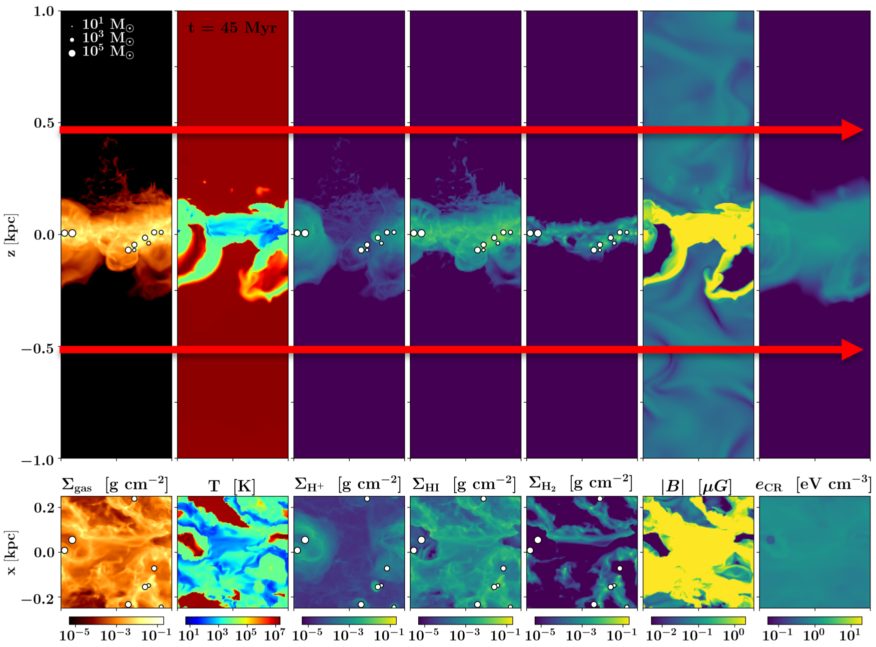
Master thesis of E. Borchert, Borchert et al., in prep.

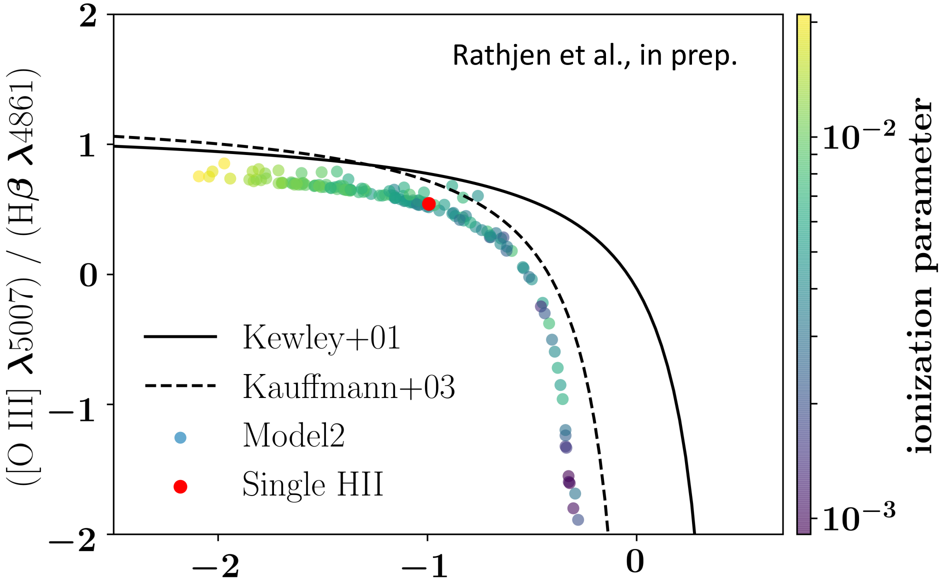
BPT Diagrams

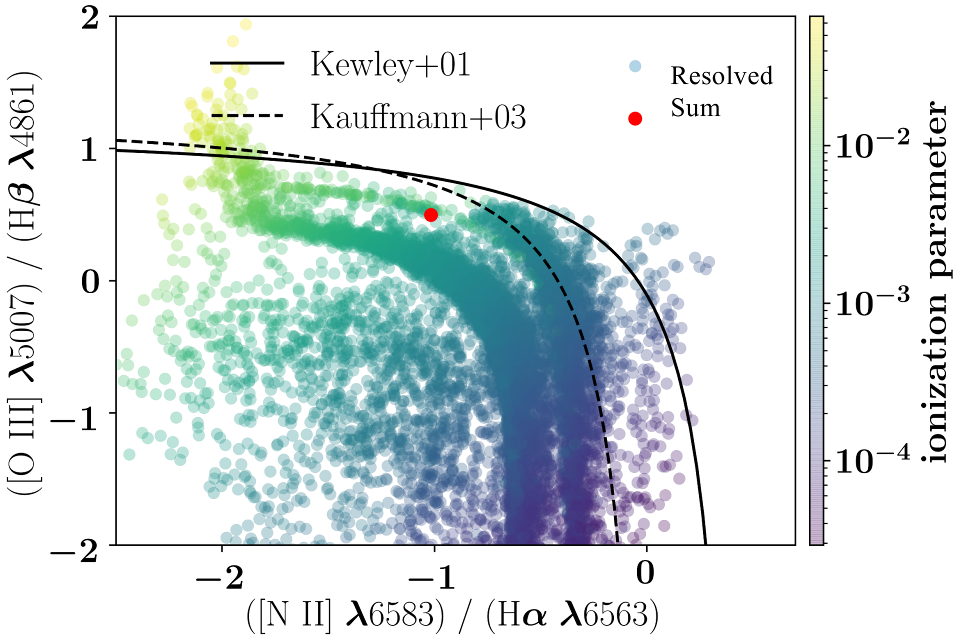
Single giant HII Region in galactic disk



Whole simulation box

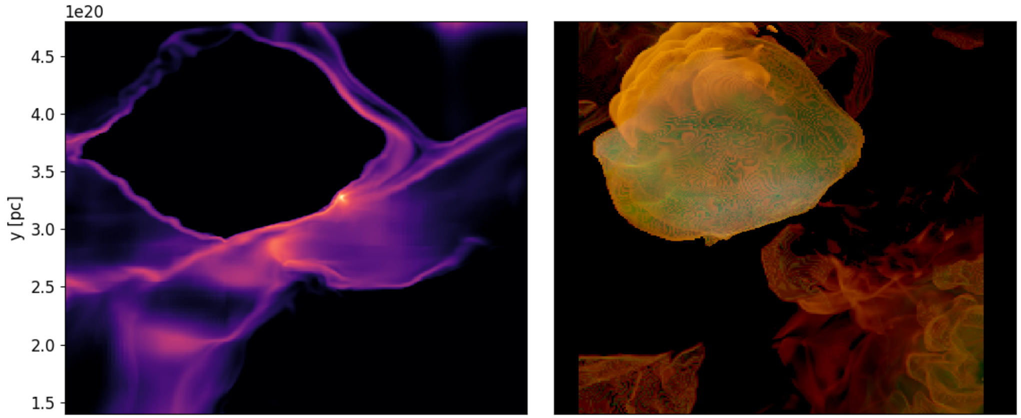


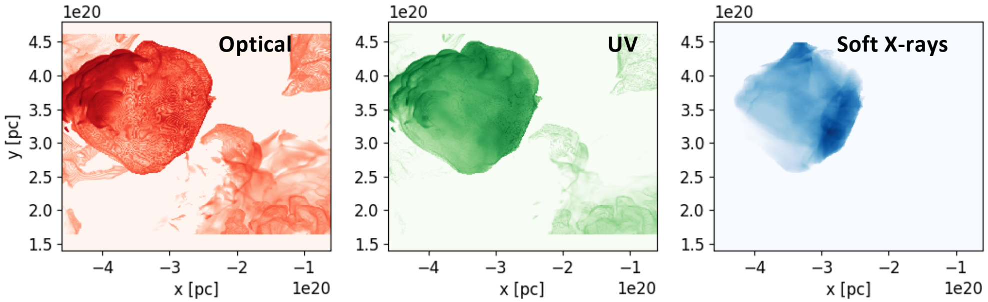




Emission from Supernova remnants

Post-processing of simulation by Seifried, SW+2018:
Supernova interacting with a molecular cloud; Synthetic emission: Mappings V



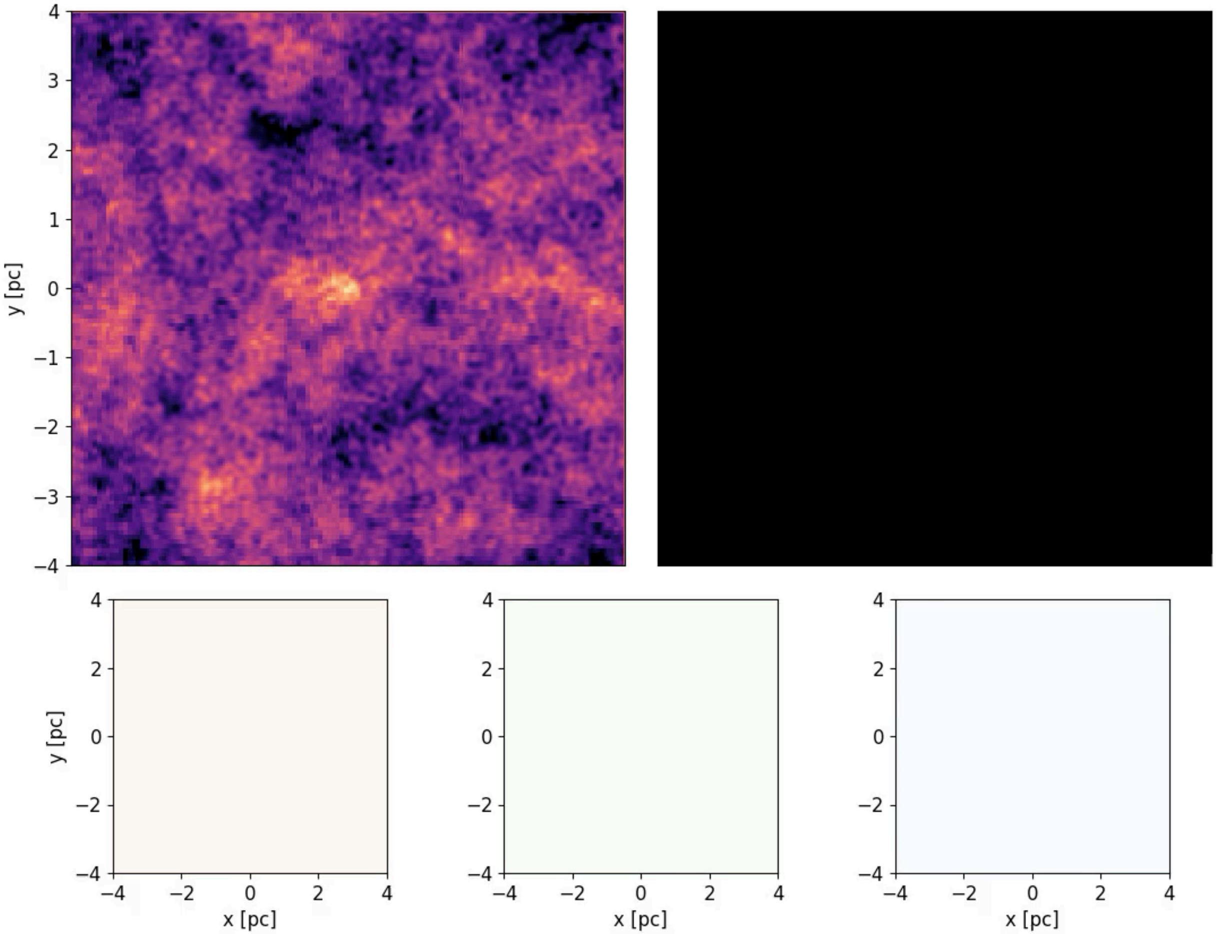


E. Makarenko, SW, S. Clarke + in prep.

Following the cooling radiation in different energy bands with MAPPINGS V (Sutherland+2018): Supernova in a fractal cloud

European Research Council

Walch, Clarke
+in prep.



Optical

UV

Soft X-rays

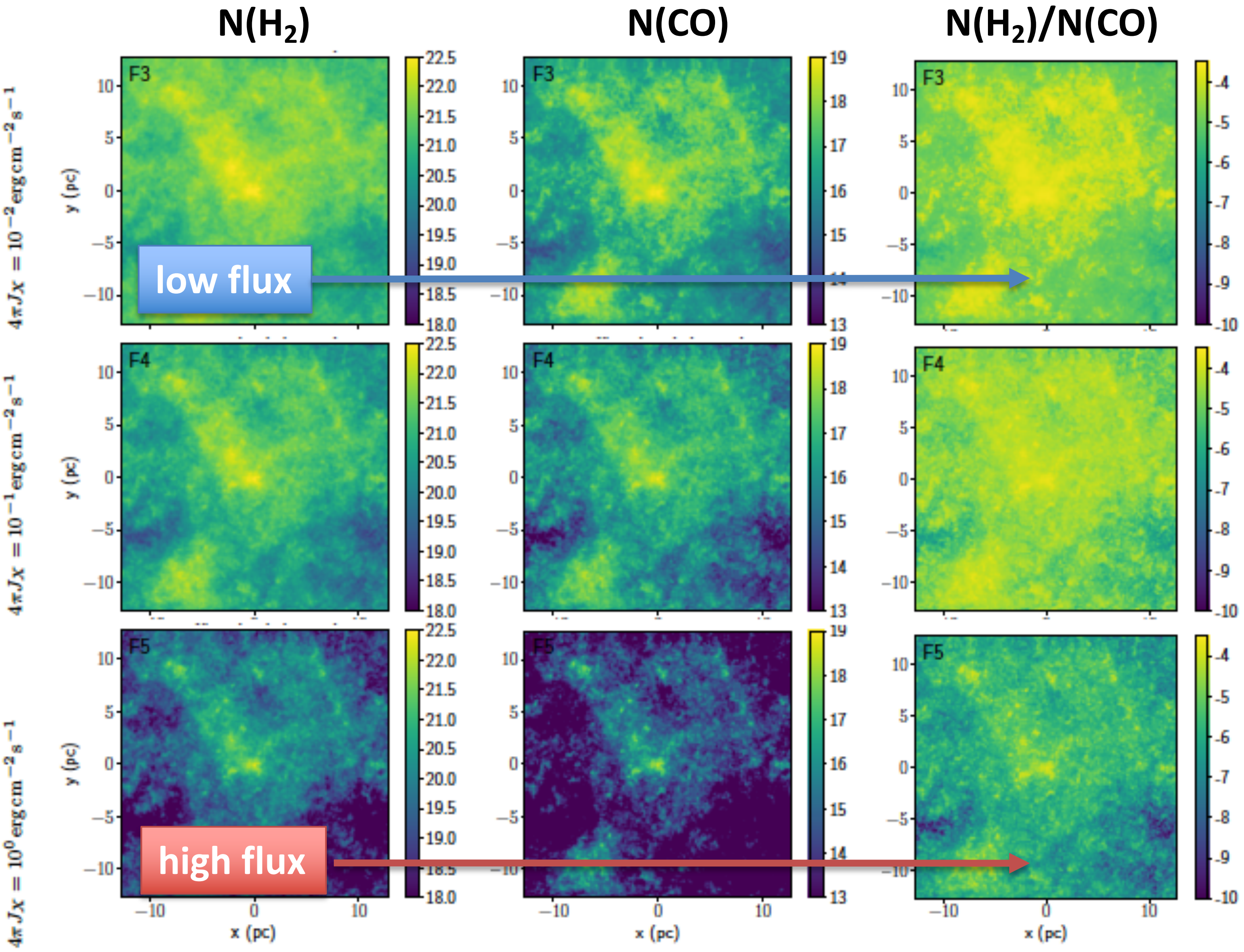
Deficit of molecular gas near strong sources of soft X-rays (e.g. X-ray flares)

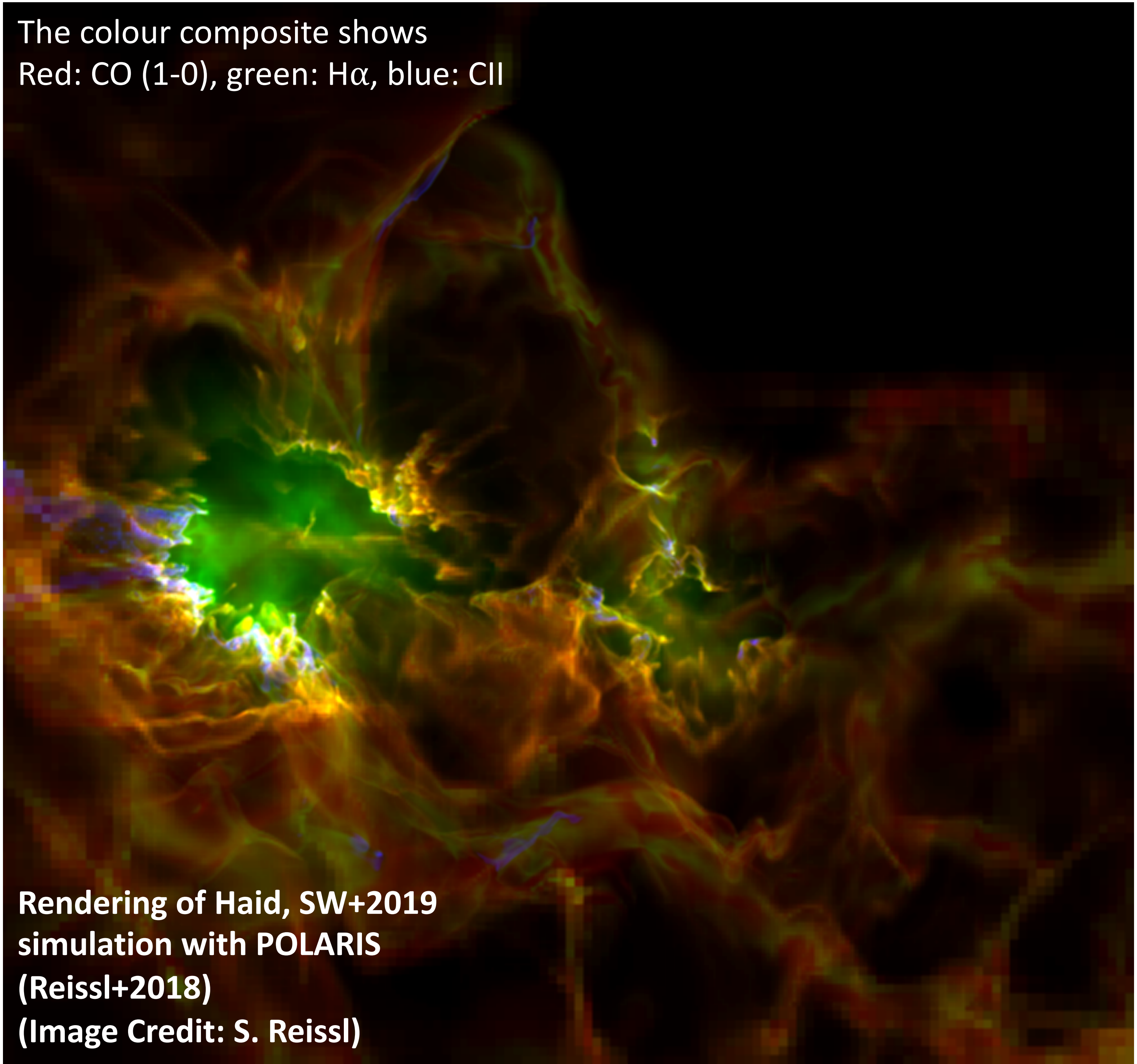
⇒We see that molecules are destroyed by X-rays

⇒They essentially have the same effect than Cosmic Rays

⇒Equilibrium models predict destruction by He⁺, but we find locally generated far-UV emission by collisions between non-thermal electrons and H_2 to dominate!

Mackey, SW+2019





The colour composite shows
Red: CO (1-0), green: Hα, blue: CII

Rendering of Haid, SW+2019
simulation with POLARIS
(Reissl+2018)
(Image Credit: S. Reissl)

Conclusions

- Apart from smart ideas: progress depends on available & future HPC technologies
- In addition: innovative software developments:
  - Efficient, hybrid parallel methods
  - New numerical algorithms, i.e. higher order schemes
  - On-the-fly data analysis?
  - Machine-learning / Neural network plugins
- Big Data: 1 snapshot 13 GB; Restart file 40 GB
  - 1 simulation: 15-20 TB
- It is essential to integrate innovative concepts, uniting physics and computing, in the teaching curriculum

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SFB 956
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DFG Priority Program 1573
ISM-SPP
Interstellar Medium

The SILCC project

GCS
Gauss Centre for Supercomputing

Thank you!!