ISM Dynamics and Star Formation

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thanks to ...

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

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... many collaborators abroad!
preface
Platon
428/427–348/347 BC

Capitoline Museum, Rome.
Plato's allegory of the cave*
Plato's allegory of the cave*

 Observatory universe

 “Demiurge”

 Ideas

 philosopher

* The Republic (514a-520a)
Plato's allegory of the cave* ↔ Astronomical observations

Laszlo Szücs, image from criticalthinking-mc205.wikispaces.com
Plato's allegory of the cave* ↔ Astronomical observations
Plato's allegory of the cave* ↔ Astronomical observations

Projection effects
Optical depth effects
Radiative transfer

→ Column density
→ Excitation / dust temperature
→ Line shift / broadening

→ Volume density
→ Temperature
→ Velocity
→ Chemical composition

Laszlo Szücs, image from criticalthinking-mc205.wikispaces.com

* The Republic (514a-520a)
Plato's allegory of the cave* ↔ Astronomical observations

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Optical depth effects
Radiative transfer

ราชการ

• Column density
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• Volume density
• Temperature
• Velocity
• Chemical composition

Inerpretation of Astronomical Data (Synthetic Observations) Assumptions from Observations Theory Experiments

*a The Republic (514a-520a)

Laszlo Szücs, image from criticalthinking-mc205.wikispaces.com
Example: from CO emission to total column density

Assumptions I.

- $I^{(12)\text{CO}}$ is optically thick
- $I^{(13)\text{CO}}$ is optically thin

Along a line of sight uniform $T_{\text{ex}}$ and same for $^{12}\text{CO}$ and $^{13}\text{CO}$

\[
T_{\text{ex}} = \frac{5.5}{\ln \left( 1 + \frac{5.5}{T_{B}^{12} + 0.82} \right)}
\]

\[
\tau_{13}(v) = -\ln \left[ 1 - \frac{T_{B}^{13}}{5.3} \left\{ \exp \left( \frac{5.3}{T_{\text{ex}}} - 1 \right)^{-1} - 0.16 \right\}^{-1} \right]
\]

\[
N^{(13)\text{CO}} = 3.0 \times 10^{14} \frac{T_{\text{ex}} \int \tau_{13}(v) dv}{1 - \exp(-5.3/T_{\text{ex}})}
\]

Assumptions II.

Uniform $N^{(12)\text{CO}}/N^{(13)\text{CO}} \sim 60^*$

$N(\text{H}_2)/N^{(12)\text{CO}}$ ratio $\sim 6.6 \times 10^3^{**}$

* Langer & Penzias (1990)
** Pineda et al. (2009)
phenomenology
M51 with Hubble (additional processing R. Gendler)
- correlation between stellar birth and large-scale dynamics
- spiral arms
- tidal perturbation from neighboring galaxy
galaxies from THINGS and HERACLES survey
(images from Frank Bigiel, ZAH/ITA)
• HI gas more extended
• H2 and SF well correlated

galaxies from THINGS and HERACLES survey (images from Frank Bigiel, ZAH/ITA)
distribution of molecular gas in the Milky Way as traced by CO emission
data from T. Dame (CfA Harvard)

Orion Nebula Cluster (ESO, VLT, M. McCaughrean)
• stars form in molecular clouds
• stars form in clusters
• stars form on \(~\) dynamical time
• (protostellar) feedback is very important
Ionizing radiation from central star $\Theta^{1}\text{C Orionis}$ Trapezium stars in the center of the ONC (HST, Johnstone et al. 1998)
• strong feedback: UV radiation from Θ1C Orionis affects star formation on all cluster scales

Trapezium stars in the center of the ONC (HST, Johnstone et al. 1998)
eventually, clusters like the ONC (1 Myr) will evolve into clusters like the Pleiades (100 Myr)
what is needed?
Star formation is intrinsically a multi-scale and multi-physics problem, where it is difficult to single out individual processes.
Star formation is intrinsically a multi-scale and multi-physics problem, where it is difficult to single out individual processes.
examples

- large scales: Kennicutt-Schmidt type relations
  - how does star formation depend on galactic environment?
- intermediate scales: molecular cloud formation
  - how to connect ISM dynamics to galactic dynamics?
- small scales: filaments and star formation
  - what is the physical origin of the ISM?

HH 901/902 in Carina with HST
global SF relations
• HI gas more extended
• H2 and SF well correlated

galaxies from THINGS and HERACLES survey
(images from Frank Bigiel, ZAH/ITA)
- standard model: roughly linear relation between H
- standard model: roughly constant depletion time: few x 10
- super linear relation between total gas and SFR

data from STING survey (Rahman et al. 2011, 2012)

• QUIZ: do you see a universal

• ANSWER: - probably not
  - in addition, the relation often is sublinear

Hierarchical Bayesian model for STING galaxies indicate varying depleting times.
physical origin of this behavior?

- maybe strong shear in dense arms (example M51, Meidt et al. 2013)...
- maybe non-star forming H column densities (recall H
physical origin of this behavior?

- maybe strong shear in dense arms (example M51, Meidt et al. 2013)...
- maybe non-star forming H column densities (recall H...
molecular cloud formation
molecular cloud formation

Idea:
Molecular clouds form at stagnation points of large-scale convergent flows, mostly triggered by global (or external) perturbations. Their internal turbulence is driven by accretion, i.e. by the process of cloud formation.

- molecular clouds grow in mass
- this is inferred by looking at molecular clouds in different evolutionary phases in the LMC (Fukui et al. 2008, 2009)

Fukui et al. (2009)
correlation with large-scale perturbations

**density/temperature fluctuations** in warm atomic ISM are caused by *thermal/gravitational instability* and/or *supersonic turbulence*

Some fluctuations are dense enough to *form H₂* within "reasonable time" → *molecular cloud*

**external perturbations** (i.e. potential changes) *increase* likelihood
star formation on *global* scales

$\tau_{H_2} \approx \frac{1.5 \text{ Gyr}}{n_H/1 \text{ cm}^{-3}}$

for $n_H \geq 100 \text{ cm}^{-3}$, $H_2$ forms within 10 Myr, this is about the lifetime of typical MC’s.

In turbulent gas, the $H_2$ fraction can become very high on short timescale

(for models with coupling between cloud dynamics and time-dependent chemistry, see Glover & Mac Low 2007a,b)

$\rho$-pdf, each shifted by $\Delta \log N = 1$

(rate from Hollenback, Werner, & Salpeter 1971)
star formation on global scales

BUT: *it doesn’t work* (at least not so easy):

*Chemistry has a memory effect!*

H$\text{2}$ forms more quickly in high-density regions as it gets destroyed in low-density parts.

mass weighted $\rho$-pdf, each shifted by $\Delta \log N=1$

(rate from Hollenback, Werner, & Salpeter 1971)

(for models with coupling between cloud dynamics and time-dependent chemistry, see Glover & Mac Low 2007a,b)
molecular cloud formation

(from Dobbs et al. 2008)
molecular cloud formation

(Dobbs & Bonnell 2007)
molecular cloud formation

molecular gas fraction of fluid element as function of time

molecular gas fraction as function of density

(Dobbs et al. 2008)
The histograms are shown for the whole LMC, and for three different regions—Bar, North, and Arc—which are indicated in the right panel.

Figure 4.

No. 1, 2009 MOLECULAR AND ATOMIC GAS IN THE LMC. II. 147

...zooming in...

In order to estimate the size of the H\textsubscript{i} envelope, we construct an H\textsubscript{i} envelope surrounding the CO emission, and then integrate the H\textsubscript{i} emission at this peak position. Next we estimate the area, the critical deviation, 0.129, for a conventional significance level. The resulting sample consists of 123 GMCs in total. Their catalog numbers and basic physical properties, taken from Fukui et al. (2008), are listed in Table 1.

For our analysis, we first selected GMCs with simple single-

In general, it is a complicated task to derive reliable physical properties of the H\textsubscript{i} gas associated with a GMC because the H\textsubscript{i} emission generally becomes much more extended than the CO. Another obstacle is that the H\textsubscript{i} line of sight, making it difficult to select the H\textsubscript{i} emission is spatially more extended than the CO emission and physically connected to a GMC. For these GMCs, we tested whether there was a bias in their location with respect to the kinematic center of the galaxy, in their CO line width or velocity range, the associated H\textsubscript{i} velocity range of 0.05, confirming that there is no selection bias.

Applied a Kolmogorov–Smirnov test to the three histograms selected GMCs compared to GMCs in the complete catalog, that there is no particular trend for these properties of the GMCs. For these GMCs, we tested that the critical deviation, 0.129, for a conventional significance level seems to be rather high for such a definition of a cloud envelope, of the H\textsubscript{i} is often elongated along the GMCs and the region of intense H\textsubscript{i} peaked H\textsubscript{i} has a less clear boundary than the CO.
image from Alyssa Goodman: COMPLETE survey
(movie from Christoph Federrath, see his talk tomorrow)
Large-eddy simulations

- We use **LES** to model the large-scale dynamics.
- Principal problem: only large scale flow properties
  - Reynolds number: \( \text{Re} = \frac{LV}{\nu} \) \((\text{Re}_{\text{nature}} \gg \text{Re}_{\text{model}})\)
  - 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?
including detailed chemistry
- Arepo and FLASH
- stochastic forcing (Ornstein-Uhlenbeck)
- self-gravity
- time-dependent chemistry (DVODE, standard variable-coefficient ordinary differential equation solver)
- cooling & heating processes
- gives you mathematically well defined boundary conditions
  --> good for statistical studies

external radiation with TreeCol (a new approximative scheme to calculate column densities from the gravity solver)
TreeCol

IDEA
• (gravitational) tree-walk
• calculated column densities
• accumulate on HEALPIX sphere

TreeCol

Figure 2. Schematic diagram illustrating the TreeCol concept. During the tree walk to obtain the gravitational forces, the projected column densities of the tree nodes (the boxes shown on the right) are mapped onto a spherical grid surrounding the particle for which the forces are being computed (the “target” particle, shown on the left). The tree already stores all of the information necessary to compute the column density of each node, the position of the node in the plane of the sky of the target particle, and the angular extent of the node. This information is used to compute the column density map at the same time that the tree is being walked to calculate the gravitational forces. Provided that the tree is already employed for the gravity calculation, the information required to create the $4\pi$ steradian map of the column densities can be obtained for minimal computational cost.

IDEA
- (gravitational) tree-walk
- calculated column densities
- accumulate on HEALPIX sphere

PERFORMANCE
- adds little computational overhead to gravitational tree-walk
- but: can add considerable memory overhead

TreeCol

**IDEA**
- (gravitational) tree-walk
- calculated column densities
- accumulate on HEALPIX sphere

**PERFORMANCE**
- adds little computational overhead to gravitational tree-walk
- but: can add considerable memory overhead
- approximation usually good to a few percent!

### TreeCol

**PERFORMANCE**
- approximation usually good to a few percent!
- example: protostellar core, comparison with RADMC

<table>
<thead>
<tr>
<th>Model</th>
<th>N$_{\text{pix}}$</th>
<th>$\theta_{\text{tol}}$</th>
<th>$\bar{\Sigma}$ [g cm$^{-2}$]</th>
<th>Error [%]</th>
</tr>
</thead>
</table>
| Spherical cloud| 3.060 $\times 10^{-3}$ | 48 0.3 3.234 $\times 10^{-3}$ | 5.7  
|                |                   | 48 0.5 3.274 $\times 10^{-3}$ | 7.0  
|                |                   | 192 0.3 3.205 $\times 10^{-3}$ | 4.7  
|                |                   | 192 0.5 3.239 $\times 10^{-3}$ | 5.8  
|                |                   | 768 0.3 3.192 $\times 10^{-3}$ | 4.3  
|                |                   | 768 0.5 3.226 $\times 10^{-3}$ | 5.4  |
| Turbulent cloud| 1.151 $\times 10^{-2}$ | 48 0.3 1.126 $\times 10^{-2}$ | 2.2  
|                |                   | 192 0.3 1.125 $\times 10^{-2}$ | 2.3  
|                |                   | 768 0.3 1.133 $\times 10^{-2}$ | 1.6  |

32 chemical species

- 17 in instantaneous equilibrium:
  - H, H₂, H³, CH⁺, CH₂⁺, OH⁺, H₂O⁺, H₃O⁺, CO⁺, HOC⁺, O⁻, C⁻ and O₂⁻

- 19 full non-equilibrium evolution
  - e⁻, H⁺, H, H₂, He, He⁺, C, C⁺, O, O⁺, OH, H₂O, CO,
    - C₂, O₂, HCO⁺, CH, CH₂ and CH₃⁺

218 reactions

Various heating and cooling processes

<table>
<thead>
<tr>
<th>Process</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Cooling:</strong></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Collisional rates (H) – Abrahamsson, Krems &amp; Dalgarno (2007)</td>
</tr>
<tr>
<td></td>
<td>Collisional rates (H(_2)) – Schroder et al. (1991)</td>
</tr>
<tr>
<td></td>
<td>Collisional rates (e(^-)) – Johnson et al. (1987)</td>
</tr>
<tr>
<td></td>
<td>Collisional rates (H(^+)) – Roueff &amp; Le Bourlot (1990)</td>
</tr>
<tr>
<td>C(^+) fine structure lines</td>
<td>Atomic data – Silva &amp; Viegas (2002)</td>
</tr>
<tr>
<td></td>
<td>Collisional rates (H(_2)) – Flower &amp; Launay (1977)</td>
</tr>
<tr>
<td></td>
<td>Collisional rates (H, T &gt; 2000 K) – Keenan et al. (1986)</td>
</tr>
<tr>
<td></td>
<td>Collisional rates (e(^-)) – Wilson &amp; Bell (2002)</td>
</tr>
<tr>
<td></td>
<td>Collisional rates (H) – Abrahamsson, Krems &amp; Dalgarno (2007)</td>
</tr>
<tr>
<td></td>
<td>Collisional rates (H(_2)) – see Glover &amp; Jappsen (2007)</td>
</tr>
<tr>
<td></td>
<td>Collisional rates (e(^-)) – Bell, Berrington &amp; Thomas (1998)</td>
</tr>
<tr>
<td></td>
<td>Collisional rates (H(^+)) – Pequignot (1990, 1996)</td>
</tr>
<tr>
<td>H(_2) rovibrational lines</td>
<td>Le Bourlot, Pineau des Forêts &amp; Flower (1999)</td>
</tr>
<tr>
<td>CO and H(_2)O rovibrational lines</td>
<td>Neufeld &amp; Kaufman (1993); Neufeld, Lepp &amp; Melnick (1995)</td>
</tr>
<tr>
<td>OH rotational lines</td>
<td>Pavlovski et al. (2002)</td>
</tr>
<tr>
<td>Gas-grain energy transfer</td>
<td>Hollenbach &amp; McKee (1989)</td>
</tr>
<tr>
<td>Recombination on grains</td>
<td>Wolfire et al. (2003)</td>
</tr>
<tr>
<td>Atomic resonance lines</td>
<td>Sutherland &amp; Dopita (1993)</td>
</tr>
<tr>
<td>H collisional ionization</td>
<td>Abel et al. (1997)</td>
</tr>
<tr>
<td>H(_2) collisional dissociation</td>
<td>See Table B1</td>
</tr>
<tr>
<td>Compton cooling</td>
<td>Cen (1992)</td>
</tr>
<tr>
<td><strong>Heating:</strong></td>
<td></td>
</tr>
<tr>
<td>Photoelectric effect</td>
<td>Bakes &amp; Tielens (1994); Wolfire et al. (2003)</td>
</tr>
<tr>
<td>H(_2) photodissociation</td>
<td>Black &amp; Dalgarno (1977)</td>
</tr>
<tr>
<td>UV pumping of H(_2)</td>
<td>Burton, Hollenbach &amp; Tielens (1990)</td>
</tr>
<tr>
<td>H(_2) formation on dust grains</td>
<td>Hollenbach &amp; McKee (1989)</td>
</tr>
<tr>
<td>Cosmic ray ionization</td>
<td>Goldsmith &amp; Langer (1978)</td>
</tr>
</tbody>
</table>
Table B2. List of photochemical reactions included in our chemical model

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>Optically thin rate (s⁻¹)</th>
<th>γ</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>166</td>
<td>H⁻ + γ → H + e⁻</td>
<td>$R_{166} = 7.1 \times 10^{-7}$</td>
<td>0.5</td>
<td>1</td>
</tr>
<tr>
<td>167</td>
<td>H₂⁺ + γ → H + H⁺</td>
<td>$R_{167} = 1.1 \times 10^{-9}$</td>
<td>1.9</td>
<td>2</td>
</tr>
<tr>
<td>168</td>
<td>H₂⁺ + γ → H + H⁺</td>
<td>$R_{168} = 5.6 \times 10^{-13}$</td>
<td>1.8</td>
<td>4</td>
</tr>
<tr>
<td>169</td>
<td>H⁺ + γ → H₂ + H⁺</td>
<td>$R_{169} = 4.9 \times 10^{-13}$</td>
<td>2.3</td>
<td>4</td>
</tr>
<tr>
<td>170</td>
<td>H⁺ + γ → H₂ + H⁺</td>
<td>$R_{170} = 4.9 \times 10^{-13}$</td>
<td>2.3</td>
<td>4</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>Rate (s⁻¹ s⁻¹)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>199</td>
<td>H + c.r. → H⁺ + e⁻</td>
<td>$R_{199} = 1.0$</td>
<td>—</td>
</tr>
<tr>
<td>200</td>
<td>He + c.r. → He⁺ + e⁻</td>
<td>$R_{200} = 1.1$</td>
<td>1</td>
</tr>
<tr>
<td>201</td>
<td>H₂ + c.r. → H⁺ + H + e⁻</td>
<td>$R_{201} = 0.037$</td>
<td>1</td>
</tr>
<tr>
<td>202</td>
<td>H₂ + c.r. → H + H⁺</td>
<td>$R_{202} = 0.22$</td>
<td>1</td>
</tr>
<tr>
<td>203</td>
<td>H₂ + c.r. → H⁺ + H⁺</td>
<td>$R_{203} = 6.5 \times 10^{-4}$</td>
<td>1</td>
</tr>
<tr>
<td>204</td>
<td>H₂ + c.r. → H⁺ + e⁻</td>
<td>$R_{204} = 2.0$</td>
<td>1</td>
</tr>
<tr>
<td>205</td>
<td>C + c.r. → C⁺ + e⁻</td>
<td>$R_{205} = 3.8$</td>
<td>1</td>
</tr>
<tr>
<td>206</td>
<td>O + c.r. → O⁺ + e⁻</td>
<td>$R_{206} = 5.7$</td>
<td>1</td>
</tr>
<tr>
<td>207</td>
<td>CO + c.r. → CO⁺ + e⁻</td>
<td>$R_{207} = 6.5$</td>
<td>1</td>
</tr>
<tr>
<td>208</td>
<td>C + γ c.r. → C⁺ + e⁻</td>
<td>$R_{208} = 2800$</td>
<td>2</td>
</tr>
<tr>
<td>209</td>
<td>CH + γ c.r. → C + H</td>
<td>$R_{209} = 4000$</td>
<td>3</td>
</tr>
<tr>
<td>210</td>
<td>CH⁺ + γ c.r. → C⁺ + H⁺</td>
<td>$R_{210} = 960$</td>
<td>3</td>
</tr>
<tr>
<td>211</td>
<td>H₂O + γ c.r. → CH₂ + e⁻</td>
<td>$R_{211} = 2700$</td>
<td>3</td>
</tr>
<tr>
<td>212</td>
<td>CH₂ + γ c.r. → CH + H⁺</td>
<td>$R_{212} = 2700$</td>
<td>3</td>
</tr>
<tr>
<td>213</td>
<td>C₂ + γ c.r. → C + C</td>
<td>$R_{213} = 1300$</td>
<td>3</td>
</tr>
<tr>
<td>214</td>
<td>OH + γ c.r. → O + H⁺</td>
<td>$R_{214} = 2800$</td>
<td>3</td>
</tr>
<tr>
<td>215</td>
<td>H₂O + γ c.r. → OH + H⁺</td>
<td>$R_{215} = 5300$</td>
<td>3</td>
</tr>
<tr>
<td>216</td>
<td>O₂ + γ c.r. → O + O</td>
<td>$R_{216} = 4100$</td>
<td>3</td>
</tr>
<tr>
<td>217</td>
<td>O₂ + γ c.r. → O₂⁺ + e⁻</td>
<td>$R_{217} = 640$</td>
<td>3</td>
</tr>
<tr>
<td>218</td>
<td>CO + γ c.r. → C + O</td>
<td>$R_{218} = 0.21 T^{1/2} z_{H_2} z_{CO}^{-1/2}$</td>
<td>4</td>
</tr>
</tbody>
</table>
HI to H2 conversion rate

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

Figure 4. Time evolution of the mass-weighted 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 et al. 2010)
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 et al. 2010)
effects of chemistry

(Glover et al. 2010)
effects of chemistry

(Glover et al. 2010)
molecular cloud formation with Arepo
molecular cloud formation

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

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Surface Density $M_\odot$ pc$^{-2}$</th>
<th>Radiation Field $G_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Milky Way</td>
<td>10</td>
<td>1</td>
</tr>
<tr>
<td>Low Density</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>Strong Field</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Low &amp; Weak</td>
<td>4</td>
<td>0.1</td>
</tr>
</tbody>
</table>

moving mesh code Arepo:
- semi-Lagrangian
- flexible refinement
- fluid instabilities and no artificial clumping
  (Agertz et al. 2007)
- can also handle sub-sonic turbulence
  (Bauer & Springel 2012)
- no preferred geometry

CO-dark gas in the Milky Way

Figure 2. Map of total column density of hydrogen nuclei for the highly resolved section of the disc in the Milky Way simulation. The gas has a range of morphologies, from dense spiral arms, to filamentary spurs, to diffuse inter-arm regions.

As an example of the results we obtain from our standard grid, we show in Figure 2 a map of the total column density in the high-resolution section of the Milky Way simulation. We see from the map that the gas exhibits very different morphologies, ranging from dense spiral arms, to filamentary spurs, to diffuse inter-arm regions. Each of these regions has a different degree of shielding to the ambient radiation field and consequently a different molecular hydrogen abundance.

Figure 3 shows the fractional abundance of molecular hydrogen relative to hydrogen in all forms as a function of column density. In this work, we define the fractional abundance of H$_2$ via the relationship

$$f_{\text{H}_2} \equiv \frac{n_{\text{H}_2}}{n}$$

where $n_{\text{H}_2}$ is the number density of hydrogen molecules and $n \equiv 2n_{\text{H}_2} + n_{\text{H}^0} + n_{\text{H}^+} + n_{\text{H}^+}$ is the total number density of hydrogen nuclei. With this definition, the maximum value of the fractional abundance is $f_{\text{H}_2} = 0.5$, corresponding to fully molecular hydrogen. Between column densities of $10^{20}$ cm$^{-2}$ and $10^{21}$ cm$^{-2}$ the molecular hydrogen begins to self-shield and its abundance rises dramatically. A similar jump in molecular hydrogen abundance is seen observationally at similar total column densities, as shown by Leroy et al. (2007) and Wolfire et al. (2008).

Gnedin et al. (2009) presented a galactic scale model of molecular hydrogen formation in which these observations were used to calibrate a clumping factor, used to account for small-scale, unresolved density fluctuations, and tuned to ensure that the model matched observations. Our results in Figure 3 are a good match to the observed transition without us having to apply any calibration factors. There is some suggestion in Figure 3 that our column densities are slightly lower for a given value of $f_{\text{H}_2}$ than some of the observational data (e.g. Savage et al. 1977). However, these observations were taken along long sight-lines within the total column density (Smith et al., 2014, MNRAS, 441, 1628).
Figure 2. Map of total column density of hydrogen nuclei for the highly resolved section of the disc in the Milky Way simulation. The gas has a range of morphologies, from dense spiral arms, to filamentary spurs, to diffuse inter-arm regions.

As an example of the results we obtain from our standard grid, we show in Figure 2 a map of the total column density in the high-resolution section of the Milky Way simulation. We see from the map that the gas exhibits very different morphologies, ranging from dense spiral arms, to filamentary spurs, to diffuse inter-arm regions. Each of these regions has a different degree of shielding to the ambient radiation field and consequently a different molecular hydrogen abundance.

Figure 3 shows the fractional abundance of molecular hydrogen relative to hydrogen in all forms as a function of column density. In this work, we define the fractional abundance of $H_2$ via the relationship $f_{H_2} \equiv \frac{n_{H_2}}{n_{\text{total}}}$, where $n_{H_2}$ is the number density of hydrogen molecules and $n_{\text{total}} \equiv 2n_{H_2} + n_{H} + n_{He}$ is the total number density of hydrogen nuclei. With this definition, the maximum value of the fractional abundance is $f_{H_2} = 0.5$, corresponding to fully molecular hydrogen. Between column densities of $10^{20}$ and $10^{21}$ cm$^{-2}$ the molecular hydrogen begins to self-shield and its abundance rises dramatically. A similar jump in molecular hydrogen abundance is seen observationally at similar total column densities, as shown by Leroy et al. (2007) and Wolfire et al. (2008).

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

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

H$_2$ column density
There is considerable variation in the abundance of H\(_2\) found in long filaments that were originally spurs connected to the disc. In the inter-arm regions molecular hydrogen is often very low, with dense filamentary structure along sight-lines perpendicular to the disc (shown by the CO column density for the highly resolved section of the disc in the Milky Way simulation). H\(_2\) is the total number density of hydrogen relative to hydrogen in all forms as a function of column density. In this work, we define the fractional abundance of H\(_2\) relative to CO column densities at some threshold, which is some suggestion in Figure 3 that our column densities in Figure 3 are a good match to the observed transition to ensure that the model matched observations. Our results were used to calibrate a clumping factor, used to account for small-scale, unresolved density fluctuations, and tune away its abundance rises dramatically. A similar jump in molecular hydrogen is the total number density of hydrogen.

The greyscale background image shows the H\(_2\) column density, with emission being above this threshold. Our dark gas fraction, estimated as described in the text, is not particularly sensitive to the choice of threshold (4). This can be attributed to their narrow filamentary geometry, many of the clouds in the inter-arm region having no portion entirely 'dark' in CO observations.

To quantify the amount of CO-dark molecular gas in our simulations, we define a dark gas fraction as a function of the choice of threshold (x). (c.f. Figure 4), while the purple points show the strength of the CO-dark gas fraction for a given value of x

\[ DG(x) = M_{CO} - M_{H_2} \]

\[ DG(x) = 3 \times 10^{-20} \text{ cm}^{-2}, \text{ for } x > 3 \]

\[ DG(x) = 3 \times 10^{-20} \text{ cm}^{-2}, \text{ for } x < 3 \]

\[ DG(x) = 3 \times 10^{-20} \text{ cm}^{-2}, \text{ for } x = 3 \]

\[ DG(x) = 3 \times 10^{-20} \text{ cm}^{-2}, \text{ for } x = 0 \]

H$_2$ forms above column densities of $10^{20}$ cm$^{-2}$

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

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

details of CO emission

relation between CO and H$_2$

Filamentary molecular clouds in inter-arm regions are likely only the observable parts of much larger structures.
46% molecular gas below CO column densities of $10^{16}$ cm$^{-2}$
42% has an integrated CO emission of less than 0.1 K km s$^{-1}$

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

dark gas fraction

Observational estimates:

Grenier et al. 2005 $f_{DG} = 0.33-0.5$
Planck collaboration 2011* $f_{DG} = 0.54$
Paradis et al. 2012* $f_{DG} = 0.62$
  inner $f_{DG} = 0.71$, outer $f_{DG} = 0.43$
Pineda et al. 2013 $f_D = 0.3$

* dust methods have large uncertainties.

other simulations

in other galaxies the dark gas fraction is likely to be higher.

Further evidence form detailed colliding flow calculations

**Figure 3.** Evolution with time of the maximum density (blue, solid line) and minimum temperature (red, dashed line) in the slow flow (top panel) and the fast flow (bottom panel). Note that at any given instant, the coldest SPH particle is not necessarily the densest, and so the lines plotted are strictly independent of one another.

**Figure 5.** The gas temperature–density distribution in the flows at the onset of star formation.


see also Pringle, Allen, Lubov (2001), Hosokawa & Inutsuka (2007)
Figure 6. Chemical evolution of the gas in the flow. In the left-hand column, we show the time evolution of the fraction of the total mass of hydrogen that is in the form of H$_2$ (red solid line) for the 6.8 km s$^{-1}$ flow (upper panel) and the 13.6 km s$^{-1}$ flow (lower panel). We also show the time evolution of the fraction of the total mass of carbon that is in the form of C$^+$ (green dashed line), C (orange dot–dashed line) and CO (blue double-dot–dashed line). In the right-hand column, we show the peak values of the fractional abundances of H$_2$ and CO. These are computed relative to the total number of hydrogen nuclei, and so the maximum fractional abundances of H$_2$ and CO are 0.5 and $1.4 \times 10^{-4}$, respectively. Again, we show results for the 6.8 km s$^{-1}$ flow in the upper panel and the 13.6 km s$^{-1}$ flow in the lower panel. Note that the scale of the horizontal axis differs between the upper and lower panels.
Figure 9. The images show the evolution of the column number density, $N$, and the velocity-integrated intensity in the $J = 1–0$ line of $^{12}$CO, $W_{\text{CO}}(1–0)$, for the region in which the first star forms in each of the flows. Four times are shown: 2 Myr prior to star formation (upper left-hand panels), 1 Myr prior to star formation (upper right-hand panels), the point of star formation (lower left-hand panels) and 0.8 Myr after the onset of star formation (lower right-hand panels). The CO-integrated intensity map is obtained via a radiative transfer calculation performed with the RADMC-3D code and uses the large velocity gradient approximation to compute the CO level populations.

We produce output snapshots every $10^5$ yr during the runs. As in the previous sections, we again see a very different picture when we compare the conditions surrounding the star-forming core in each flow. The main difference between the simulations is that the slow flow is almost entirely Jeans unstable by the onset of star formation (i.e. its gravitational energy is greater than its thermal energy), while the fast flow is in general gravitationally stable. This 33

summary
summary

- hierarchical Bayesian statistics indicated galaxy to galaxy variations in the KS relation with typically sublinear slope
  → *is there lots of diffuse CO gas in galaxies?*

- detailed (M)HD calculations with time-dependent chemistry allow us to study the properties of CO-dark H$_2$ gas
  → *implications for interpreting observational data?*

- molecular clouds are filamentary, but the filament parameters (width, slope, central density) may vary significantly
  → *what does it mean for star cluster formation?*

- next steps: *improved multi-scale and multi-physics simulations with Arepo and FLASH*
thanks