Improved ISM Modelling in Simba

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What is Simba?

- Smoothed-particle hydrodynamics simulation suite (GIZMO)
- Galaxy formation & evolution
- Advanced sub-grid modelling (BH feedback, winds etc.)
- Chemistry and cooling is off-loaded to Grackle



Updating Simba's star formation



Why?



(Data from Bouwens et al., 2015)

What affects star formation?



Primarily:

Molecular hydrogen drives star formation

Secondary Processes:

- 1. Dust catalyses the formation of molecular hydrogen
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Star Formation Rate



Star Formation Rate

How do we calculate the molecular hydrogen fraction?



The Setup:

- Spherical cloud of gas
- Exposed to isotropic, dissociating radiation field
- Assume atomic to molecular transition occurs in infinitely thin shell

The Inputs:

- Metallicity
- Dust column density

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Computationally fast

Very simple

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Chemical Network

The Setup:

- Add three new chemical species to the network in Grackle: H^{+} , H_{2} , H_{2}^{+}
- Pass the abundance of each species to Simba

	Reaction				
The C	$H + e^{-}$	\rightarrow	$H^- + \gamma$		
	$H^- + H$	\rightarrow	$H_2 + e^-$		
•	$H + H^+$	\rightarrow	$H_2^+ + \gamma$		
•]	$H_{2}^{+} + H$	\rightarrow	$H_2 + H^+$	cia	
	$H_2 + H^+$	\rightarrow	$H_{2}^{+} + H$		
•	$H_2 + e^-$	\rightarrow	$H + H + e^{-}$	ar	
Ĵ	$H_2 + H$	\rightarrow	H + H + H	r th	
	$H^{-} + e^{-}$	\rightarrow	$\mathrm{H} + \mathrm{e}^{-} + \mathrm{e}^{-}$	v u	
	$H^- + H$	\rightarrow	$H + e^- + H$		
	$H^- + H^+$	\rightarrow	H + H		
The I	$H^- + H^+$	\rightarrow	$H_2^+ + e^-$		
	$H_{2}^{+} + e^{-}$	\rightarrow	H + H		
•	$H_{2}^{+} + H^{-}$	\rightarrow	$H_2 + H$		
•]	H + H + H	\rightarrow	$H_2 + H$		
	$H + H + H_2$	\rightarrow	$H_2 + H_2$		
	$H^- + \gamma$	\rightarrow	$H + e^{-}$		
	$H_2^+ + \gamma$	\rightarrow	$H + H^+$		
comp	$H_2 + \gamma$	\rightarrow	$H_2^+ + e^-$		
	$H_2^+ + \gamma$	\rightarrow	$H^+ + H^+ + e^-$		
Very s	$H_2 + \gamma$	\rightarrow	H + H		
	H + H + grain	\rightarrow	$H_2 + grain$		

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' thin

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Н	eactic	n
$H + e^{-}$	î	$H^- + \gamma$
H- + H	î	$H_2 + e^-$
$H + H^+$	Ŷ	$H_{2}^{+} + \gamma$
$H_{2}^{+} + H$	Ŷ	$H_2^2 + H^+$
$H_2^2 + H^+$	Ŷ	$H_{2}^{+} + H$
$H_2 + e^-$	î	$H + H + e^{-}$
$H_2 + H$	Ŷ	H + H + H
$H^{-} + e^{-}$	Ŷ	$H + e^- + e^-$
H- + H	Ŷ	$H + e^- + H$
$H^{-} + H^{+}$	Î	H + H
$H^{-} + H^{+}$	î	$H_{2}^{+} + e^{-}$
$H_{2}^{+} + e^{-}$	î	H_+H
$H_{2}^{+} + H^{-}$	î	$H_2 + H$
H + H + H	Î	$H_2 + H$
$H + H + H_2$	Î	$H_2 + H_2$
$H^{-} + \gamma$	î	$H + e^{-}$
$H_{2}^{+} + \gamma$	î	$H + H^+$
$H_2^{-} + \gamma$	î	$H_2^+ + e^-$
$H_{2}^{+} + \gamma$	î	$H^{+} + H^{+} + e^{-}$
$H_2^{-} + \gamma$	î	H + H
H + H + grain	Î	$H_2 + grain$

Explicitly solves chemistry for each particle

Much slower than KMT

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Molecule dissociates from dust

Grain-atom collision

Η



Atom "sticks" to dust

Η



Dust column density is an input to the KMT model

No specific models for different formation pathways

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	R	eactio	on		<u>Olackie</u>	
Dust c he KN No spe ormat	$\begin{array}{c} H + e^{-} \\ H^{-} + H \\ H + H^{+} \\ H_{2}^{+} + H \\ H_{2}^{+} + H \\ H_{2}^{+} + e^{-} \\ H_{2}^{+} + H \\ H^{-} + e^{-} \\ H^{-} + H \\ H^{-} + H^{+} \\ H^{-} + H^{+} \\ H^{-} + H^{+} \\ H_{2}^{+} + e^{-} \\ H_{2}^{+} + H^{-} \\ H_{2}^{+} + H^{-} \\ H + H + H \\ H + H + H_{2} \\ H^{-} + \gamma \\ H_{2}^{+} + \gamma \\$	<u>↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑</u>	$H^{-} + \gamma$ $H_{2} + e^{-}$ $H_{2}^{+} + \gamma$ $H_{2} + H^{+}$ $H_{2}^{+} + H$ $H + H + e^{-}$ $H + H + H$ $H + e^{-} + e^{-}$ $H + e^{-} + H$ $H_{2}^{+} + e^{-}$ $H + H$ $H_{2}^{+} + H$ $H_{2} + H$ $H_{3} + H$	put to	Explicit colculation	Grain "sticking" potential \int $S(T, T_{grain})$
	$H_2 \neq \gamma$ $H_2^+ + \gamma$	\rightarrow	$H_2 + C$ $H^+ + H^+ + e^-$		accurate!	
	H + H + grain	\rightarrow	H_2 + grain			

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Dust Growth and Destruction

Grains grow through accretion of gas-phase metals

M

Dust Growth and Destruction



Dust Growth and Destruction



<u>Simba</u>

Growth and destruction rates characterised by timescales:

$$\left(\frac{dM_{grain}}{dt}\right)_i \propto \frac{1}{\tau_i}$$

The accretion timescale:

$$\tau_{accr} = \tau_{ref} \left(\frac{T_{ref}}{T_{gas}} \right) \left(\frac{\rho_{ref}}{\rho_{gas}} \right) \left(\frac{Z_{\odot}}{Z_{gas}} \right)$$

Reference parameters are tuned:

$$T_{ref} = 20 \text{ K}$$

<u>Simba</u>

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Our Work

Solve gas-grain heat balance for dust temperature: Rate of heat transfer between gas and dust Grain opacity $4\sigma T_{gr}^4 \kappa_{gr}^{\bullet} = 4\sigma T_{CMB}^4 \kappa_{gr} + \Lambda_{gas-grain}$ Radiative Heating cooling **Replace reference temperature:** $\tau_{accr} = \tau_{ref} \left(\frac{T_{gr}}{T_{aas}} \right) \left(\frac{\rho_{ref}}{\rho_{aas}} \right) \left(\frac{Z_{\odot}}{Z_{aas}} \right)$

Dust model integrated into chemical network

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Isolated Case

Solve gas-grain heat balance for dust temperature:



Replace reference temperature:

$$\tau_{accr} = \tau_{ref} \left(\frac{T_{gr}}{T_{gas}} \right) \left(\frac{\rho_{ref}}{\rho_{gas}} \right) \left(\frac{Z_{\odot}}{Z_{gas}} \right)$$

Dust model integrated into chemical network

External Radiation Field

Interstellar radiation field heats dust:

$$4\sigma T_{gr}^{4}\kappa_{gr} = 4\sigma T_{CMB}^{4}\kappa_{gr} + \Lambda_{gas-grain} + \Gamma_{ISRF}G_{0}$$
Dust heating rate
ISRF strengt

Estimate ISRF from star formation in local environment:



What affects star formation?



Modelling Changes

- Removal of KMT model left star formation unresolved
- Implement sub-grid model to fix this:
 - 1. Gas reaches sufficiently high density \rightarrow Treat as two phases
 - Only cool the molecular phase → Update its density to maintain pressure equilibrium



Our Simulations

- Two production simulations completed on Cirrus:
 - 50 Mpc/h box 1024³ particles
 - 25 Mpc/h box 1024³ particles
- Evolved from redshift 99 to 6

Mass Functions: SFR



25 Mpc/h

Molecular Hydrogen Fraction



(25 Mpc/h)

Dust-to-Gas Ratio



 $\log_{10} (Z/Z_{\odot})$



Dust Temperature

• Contours containing 10%, 50%, 80% and 95% of the data

Summary

What we've done

Improvements:

- Extended chemical network
- Solving for dust temperature
- Molecular hydrogen calculation Additions:
 - ISRF model
 - Two-phase sub-grid model

What's next?

- Run to lower redshifts
- Comparison to new observational data
- Higher resolutions (zooms)





What we've seen

- Good agreement with fiducial Simba
- Improved SFR
- Interesting results to look into!

Dust Heating Rate



Dust-to-Metal Ratio



