# Molecule formation in turbulent gas

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# Key questions

- How quickly do molecular clouds form?
- How is the molecular gas distributed?
- What role does supersonic turbulence play?

# Simulations

- ZEUS-MP v1 - MHD, self-gravity (periodic BCs)
- Detailed atomic cooling function
- Simple hydrogen chemistry
- Highly approximate treatment of shielding

# Chemistry

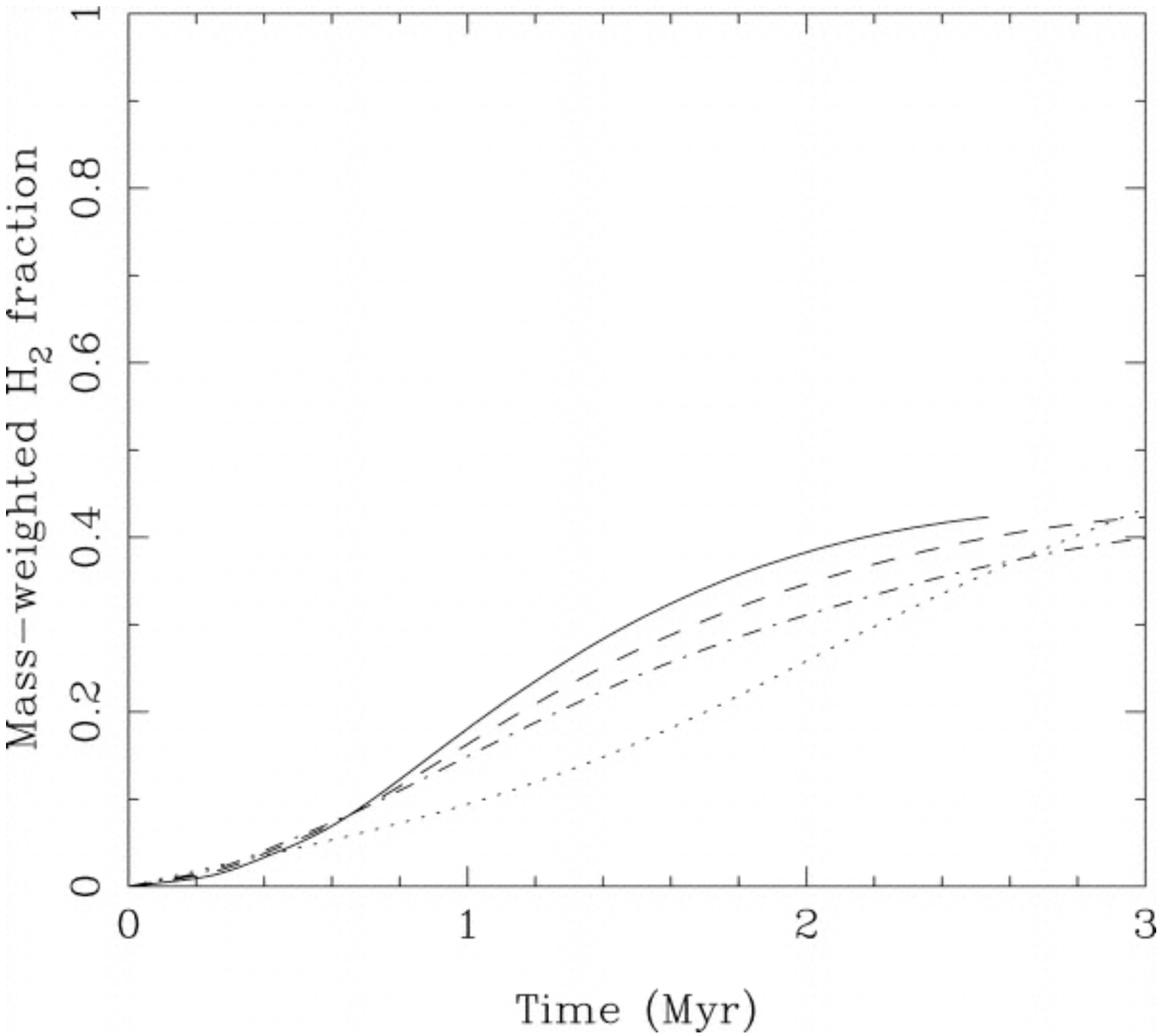
- $H_2$ formation on dust grains
- $H_2$ collisional dissociation
- $H_2$ photodissocation
- H ionization (collisional, cosmic rays)
- $H^+$ recombination (gas-phase, grains)

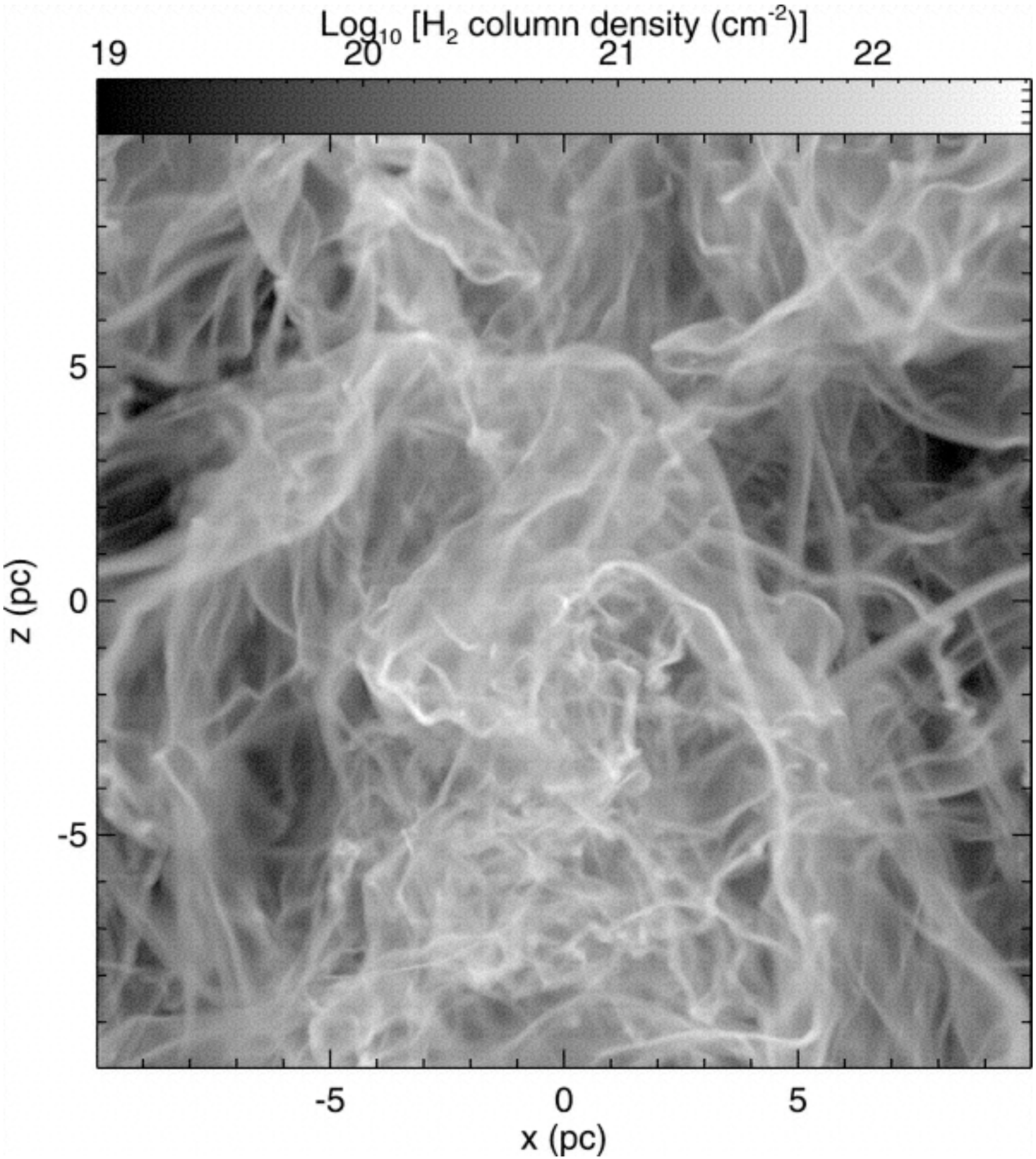
# Shielding

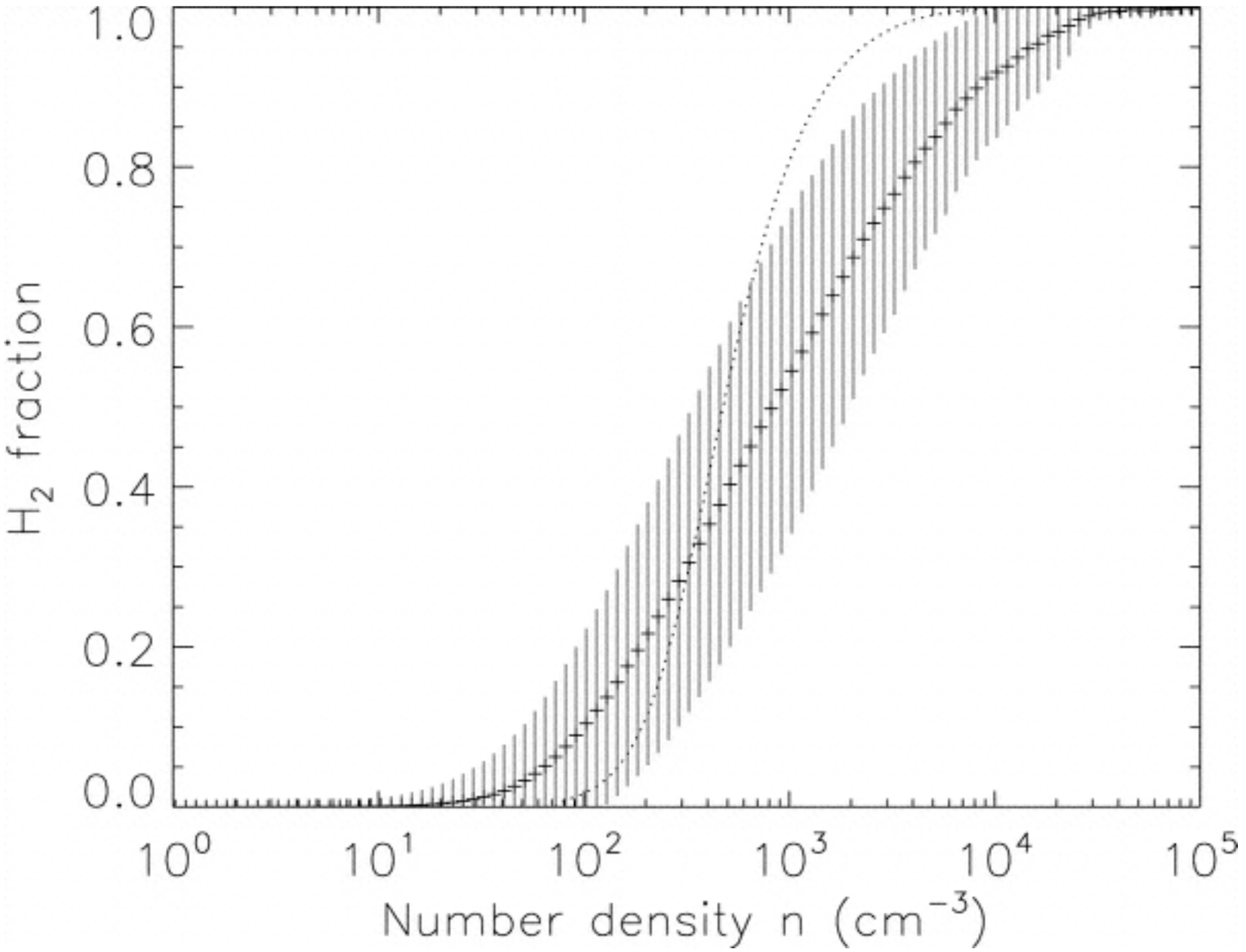
- Two forms of shielding: $H_2$ self-shielding, dust
- Accurate treatment computationally prohibitive, so use very simple approximations
- Local approximation: only gas within the grid cell contributes
- Six-ray approximation: ray-tracing along coordinate axes of simulation volume

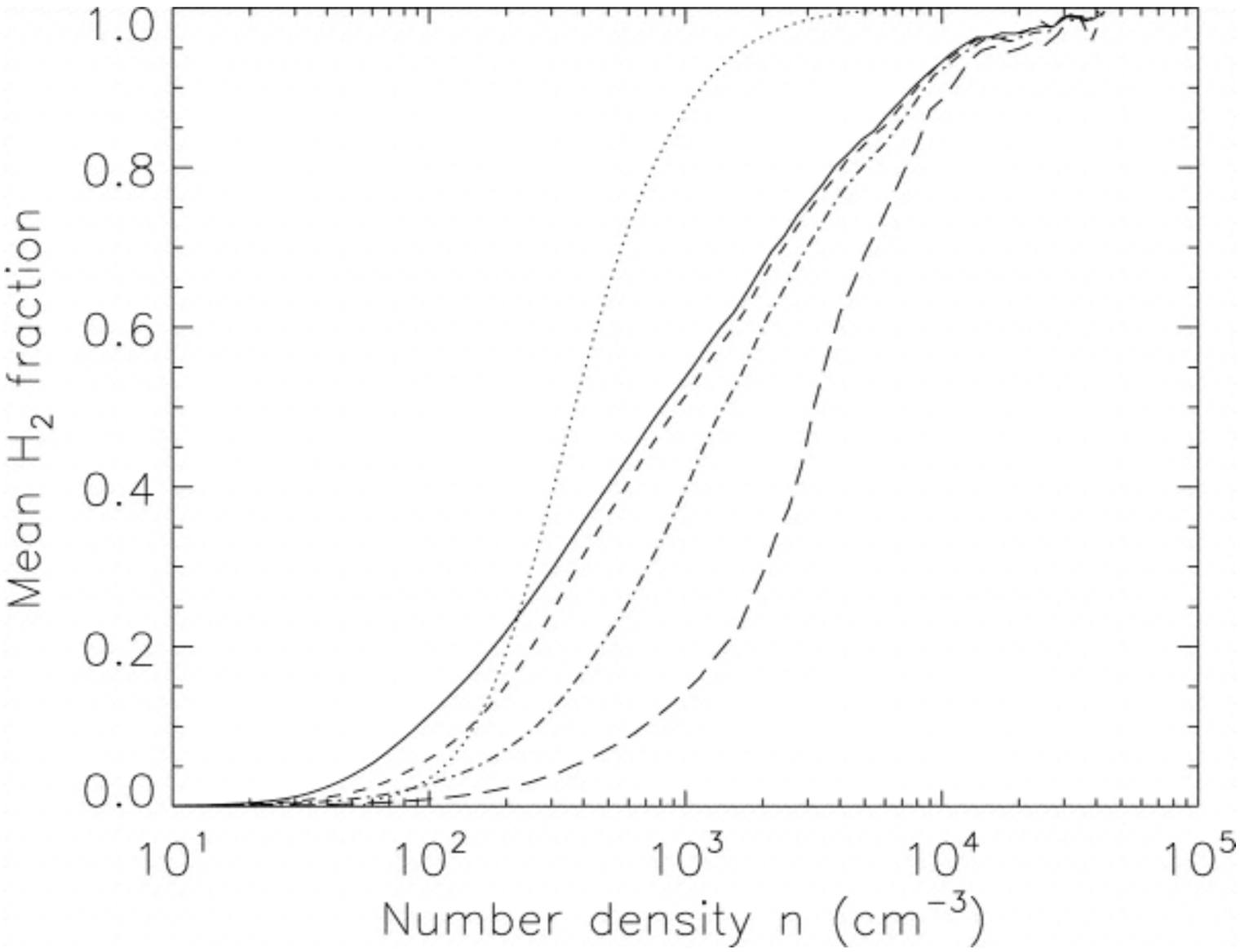
# Simulation details

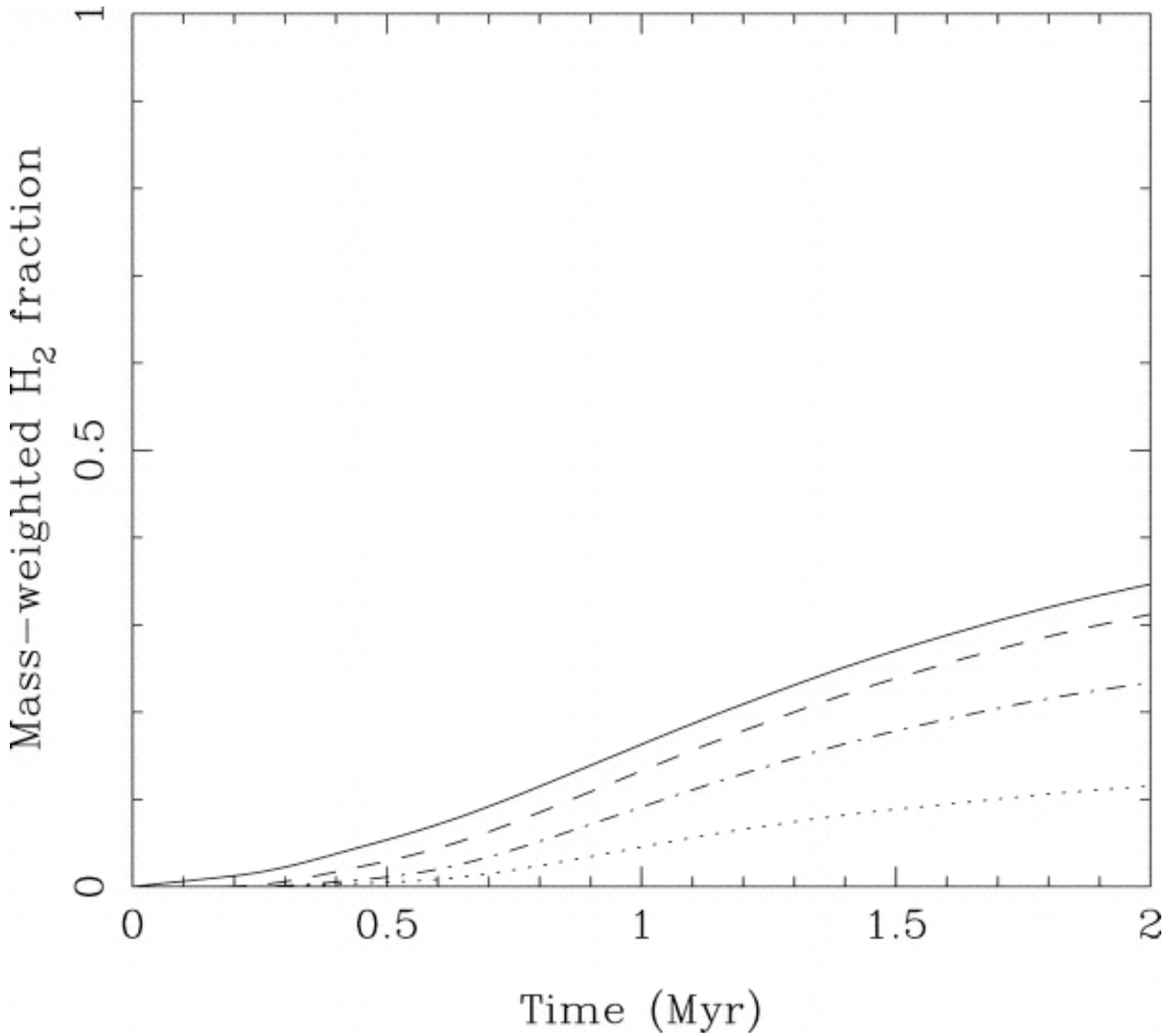
- Resolution: $64^3$, $128^3$, **$256^3$**, $512^3$
- Box size: **20**, 40, 60 pc
- Density: 10, 30, **100** $cm^{-3}$
- Velocity: 1.0, 2.5, 5.0, **10.0** $kms^{-1}$
- Magnetic field: 0.0, **5.85**, 11.7, 23.4, 58.5 μG

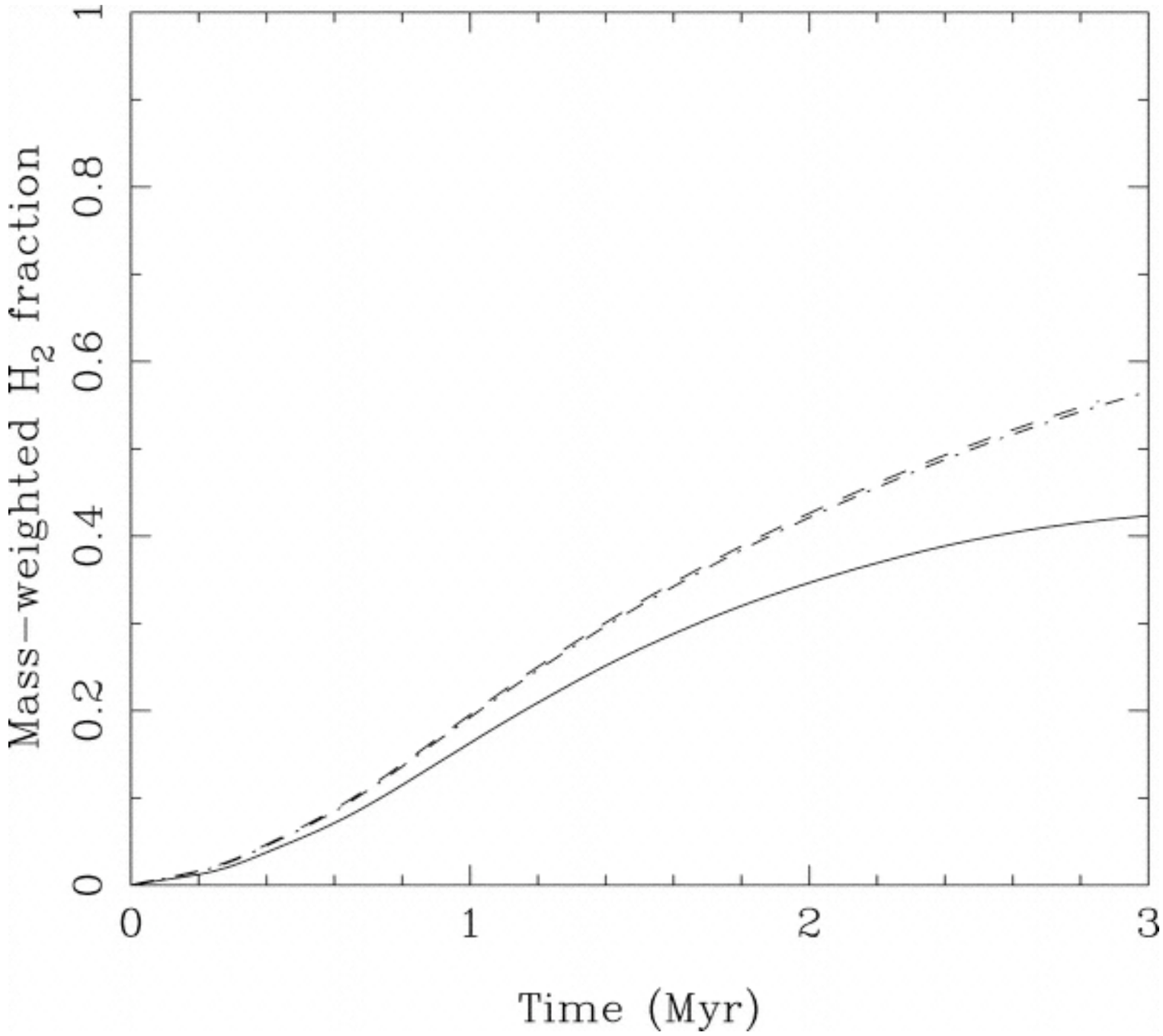

Mass−weighted $H_2$ fraction
0
0.2
0.4
0.6
0.8
1
0
1
2
3
Time (Myr)

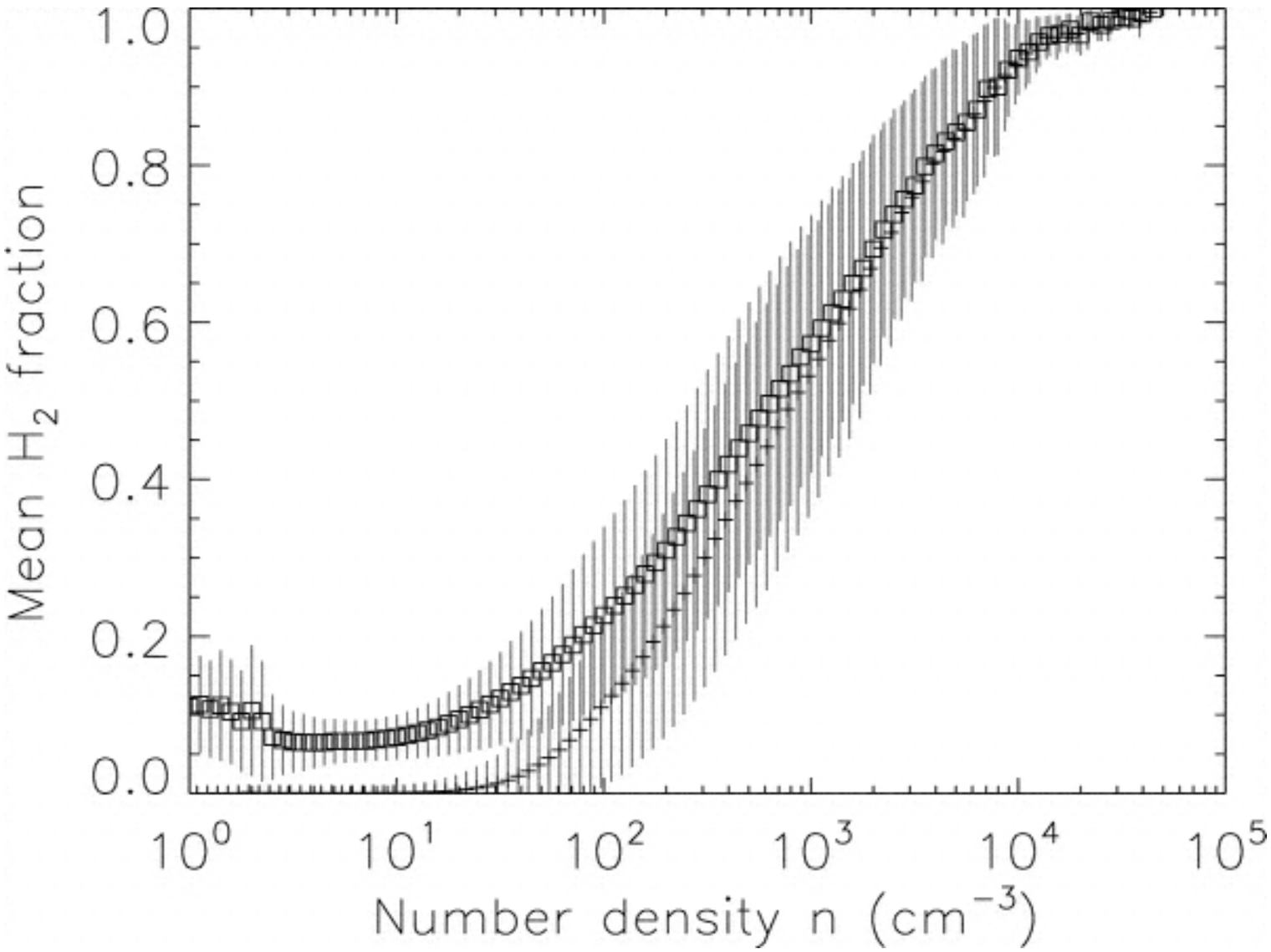

Log10 [H2 column density (cm-2)]
19
20
21
22
5
0
-5
z (pc)
-5
0
5
x (pc)

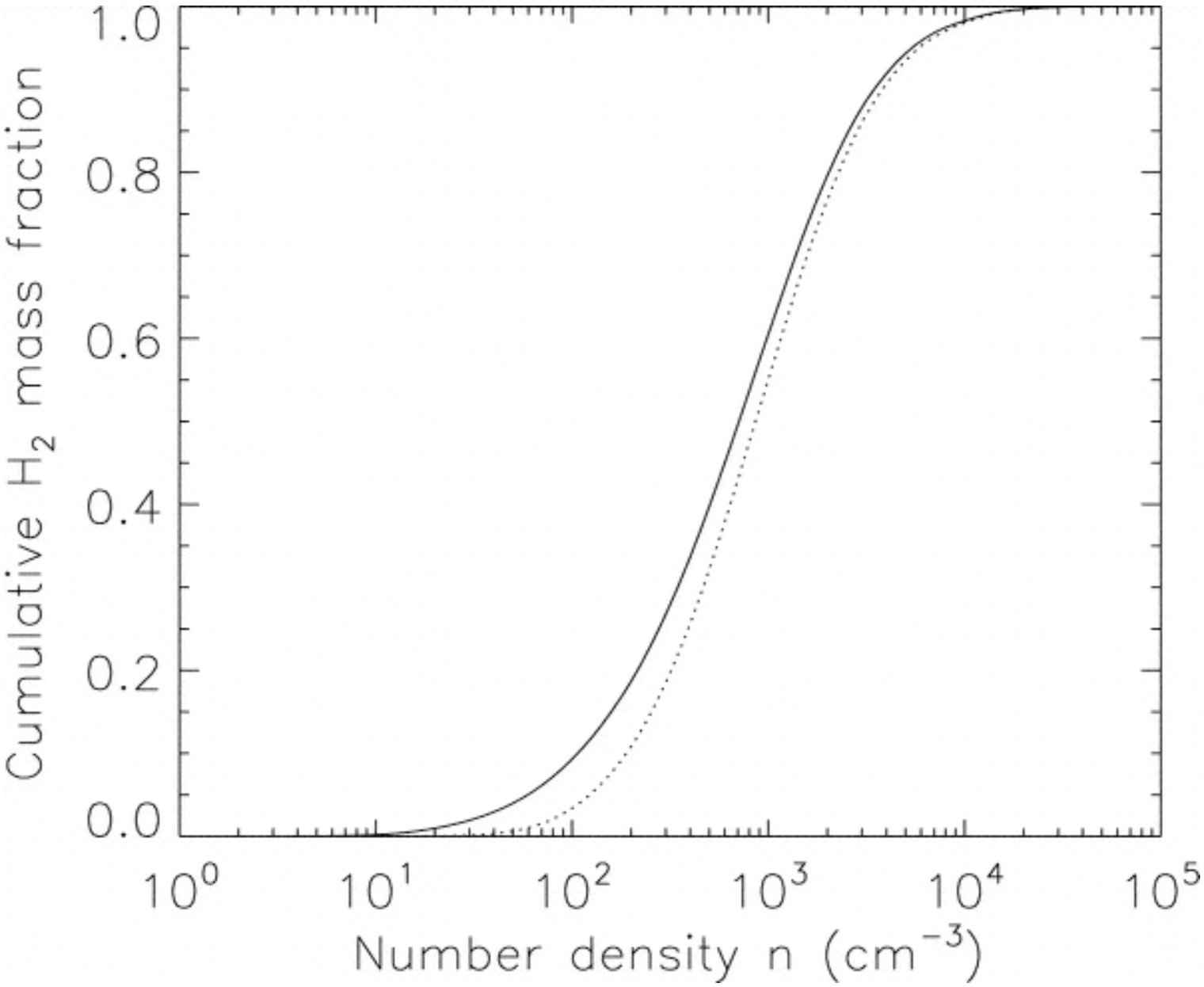

1.0
0.8
0.6
0.4
0.2
0.0
$H_2$ fraction
$10^0$
$10^1$
$10^2$
$10^3$
$10^4$
$10^5$
Number density n ($cm^{-3}$)

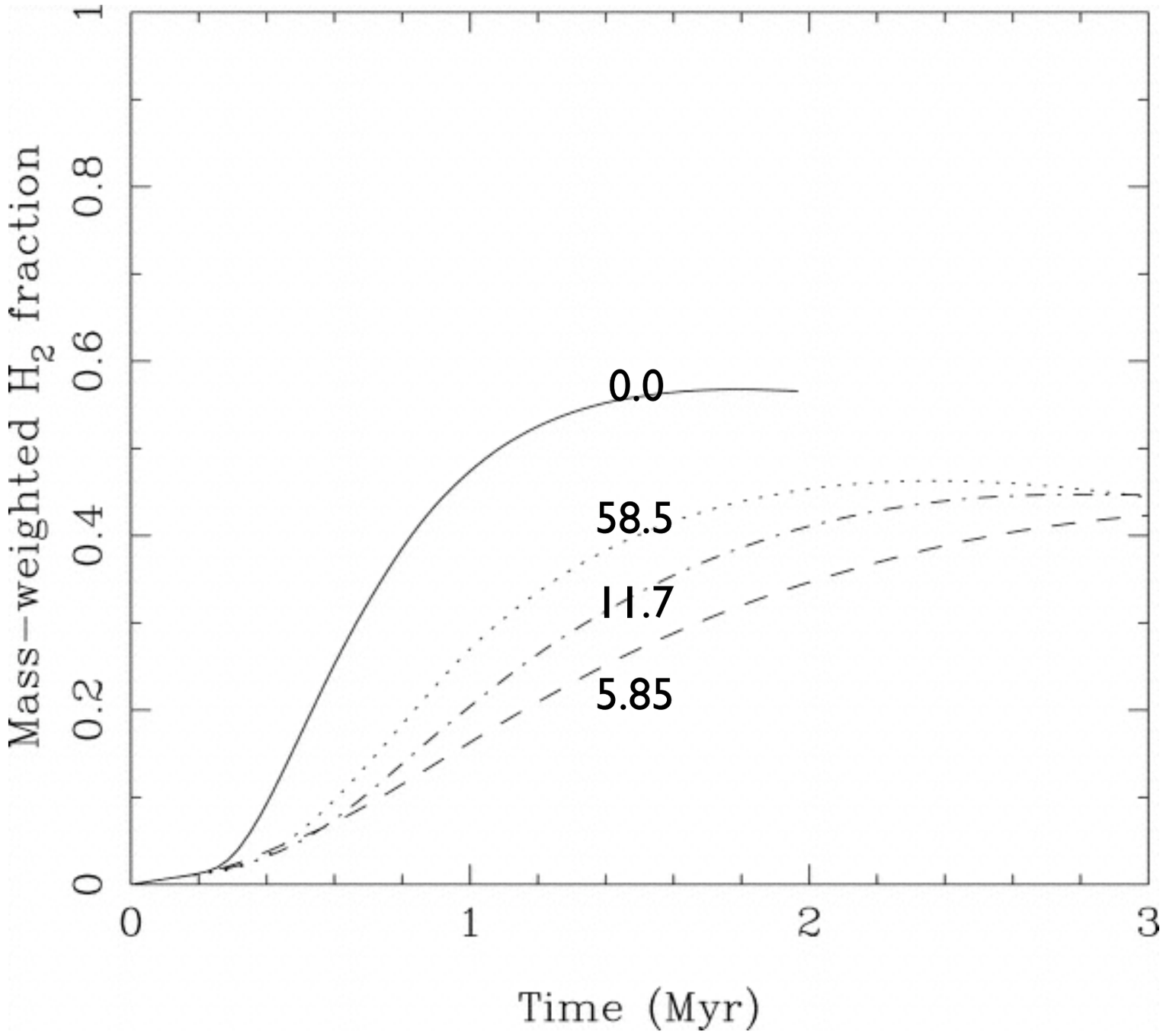

1.0
0.8
0.6
0.4
0.2
0.0
Mean $H_2$ fraction
$10^1$
$10^2$
$10^3$
$10^4$
$10^5$
Number density n ($cm^{-3}$)

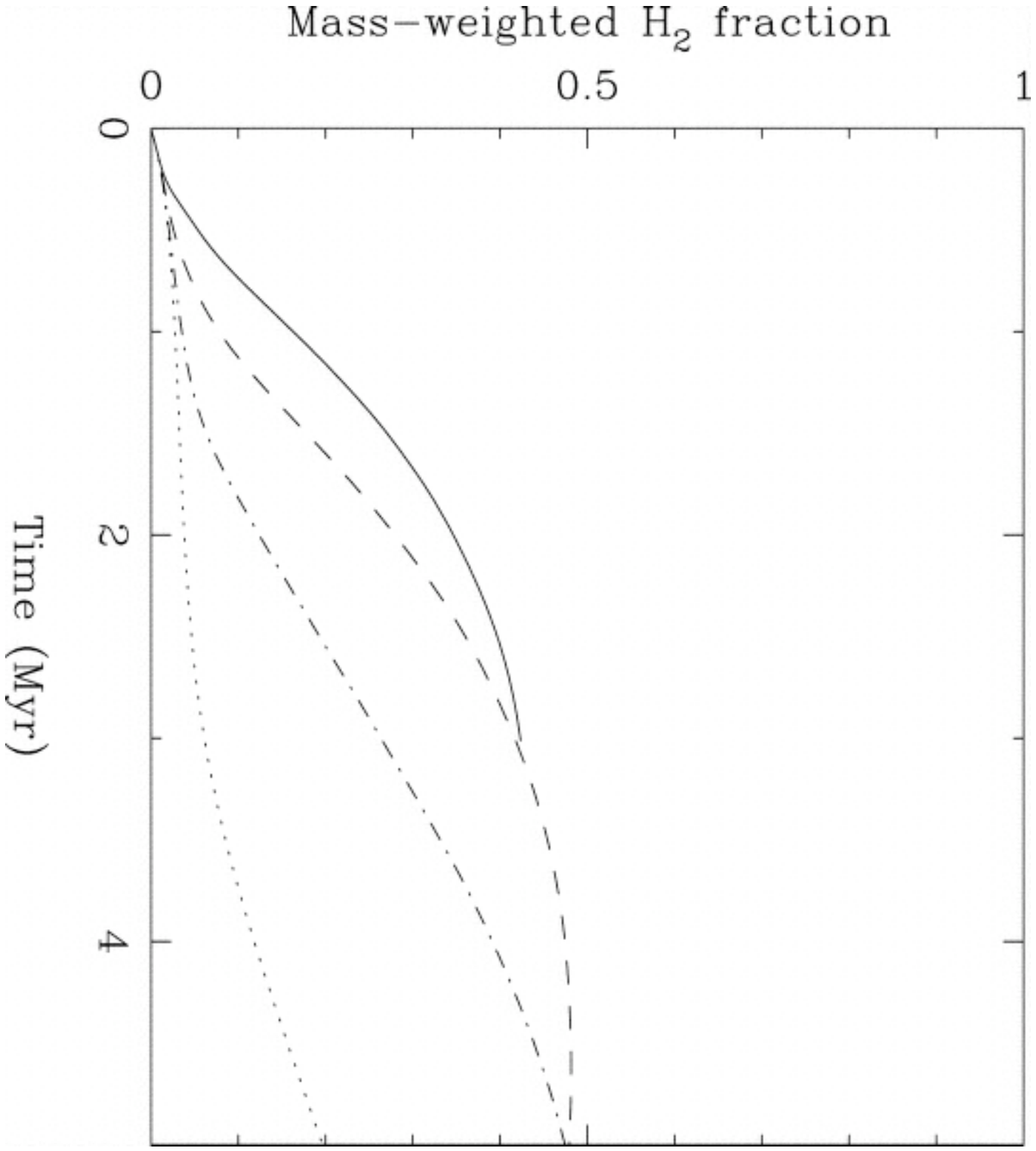

Mass−weighted $H_2$ fraction
0
0.5
1
0
0.5
1
1.5
2
Time (Myr)

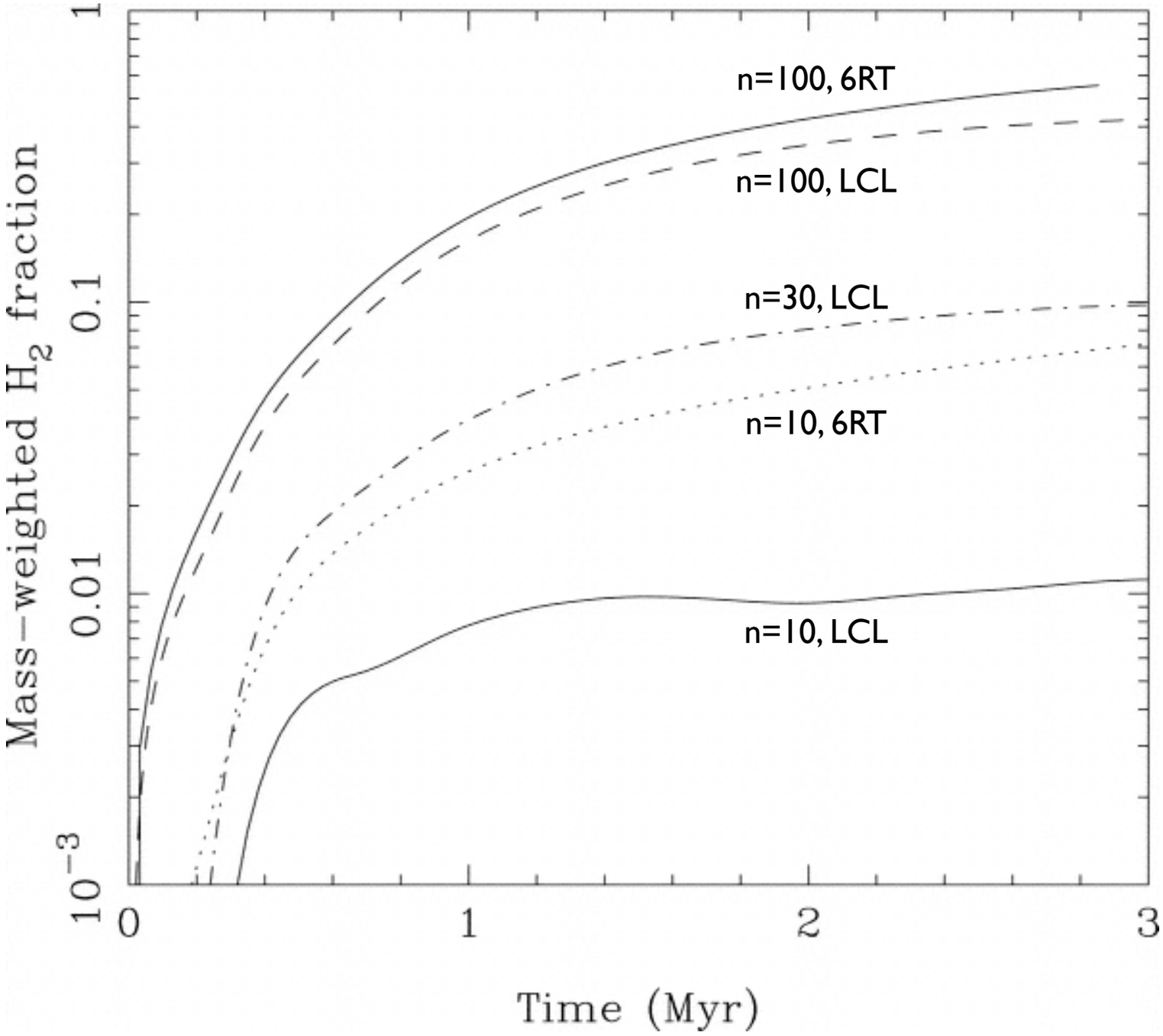

Mass−weighted $H_2$ fraction
0
0.2
0.4
0.6
0.8
1
0
1
2
3
Time (Myr)


1.0
0.8
0.6
0.4
0.2
0.0
Mean H2 fraction
10^0
10^1
10^2
10^3
10^4
10^5
Number density n (cm^-3)


1.0
0.8
0.6
0.4
0.2
0.0
Cumulative $H_2$ mass fraction
$10^0$
$10^1$
$10^2$
$10^3$
$10^4$
$10^5$
Number density n ($cm^{-3}$)


Mass−weighted $H_2$ fraction
0
0.2
0.4
0.6
0.8
1
0
1
2
3
Time (Myr)
0.0
58.5
11.7
5.85


Mass−weighted $H_2$ fraction
0
0.5
1
0
2
4
Time (Myr)

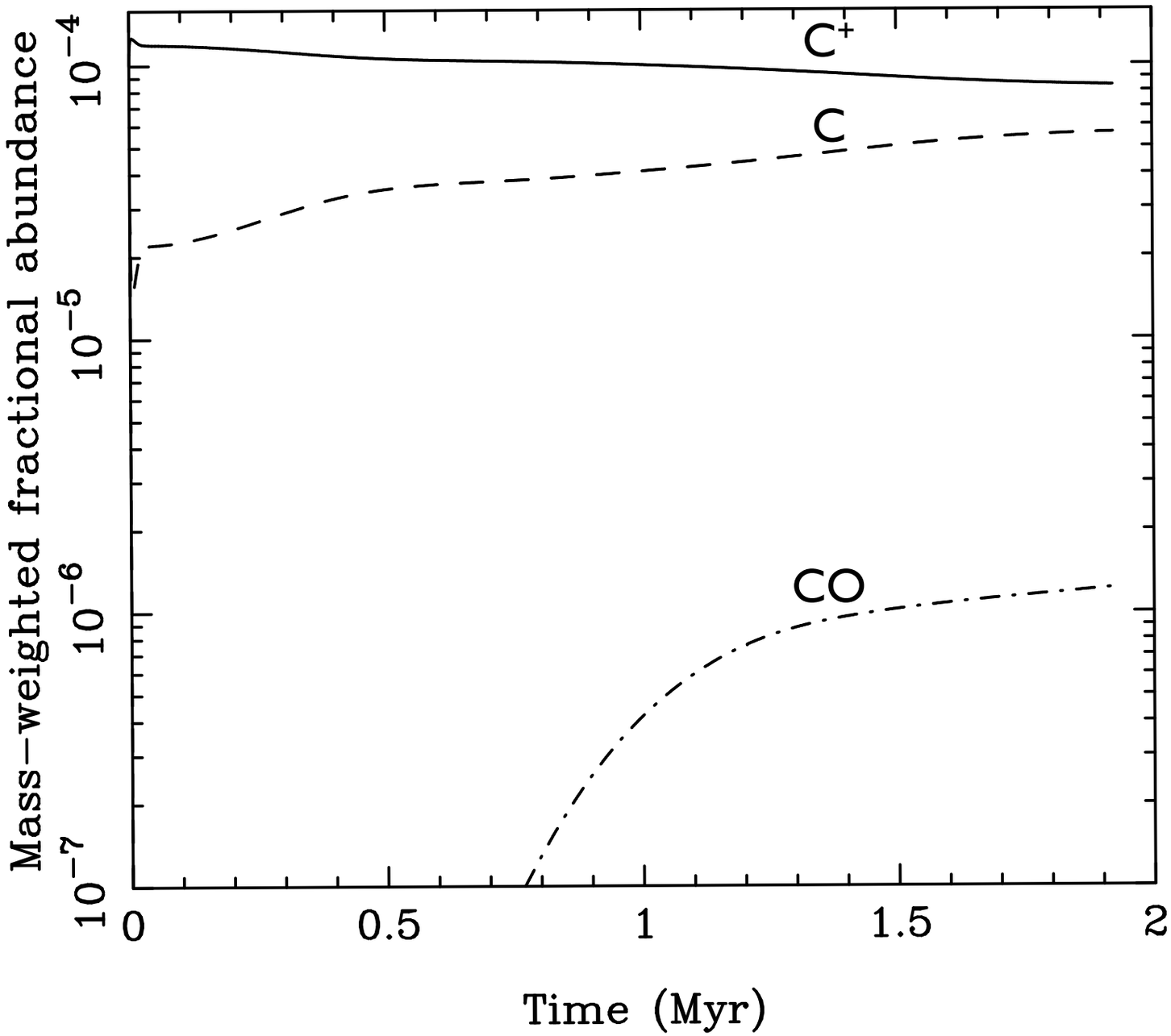

n=100, 6RT
n=100, LCL
n=30, LCL
n=10, 6RT
n=10, LCL
Mass−weighted $H_2$ fraction
Time (Myr)
1
0.1
0.01
$10^{-3}$
0
1
2
3

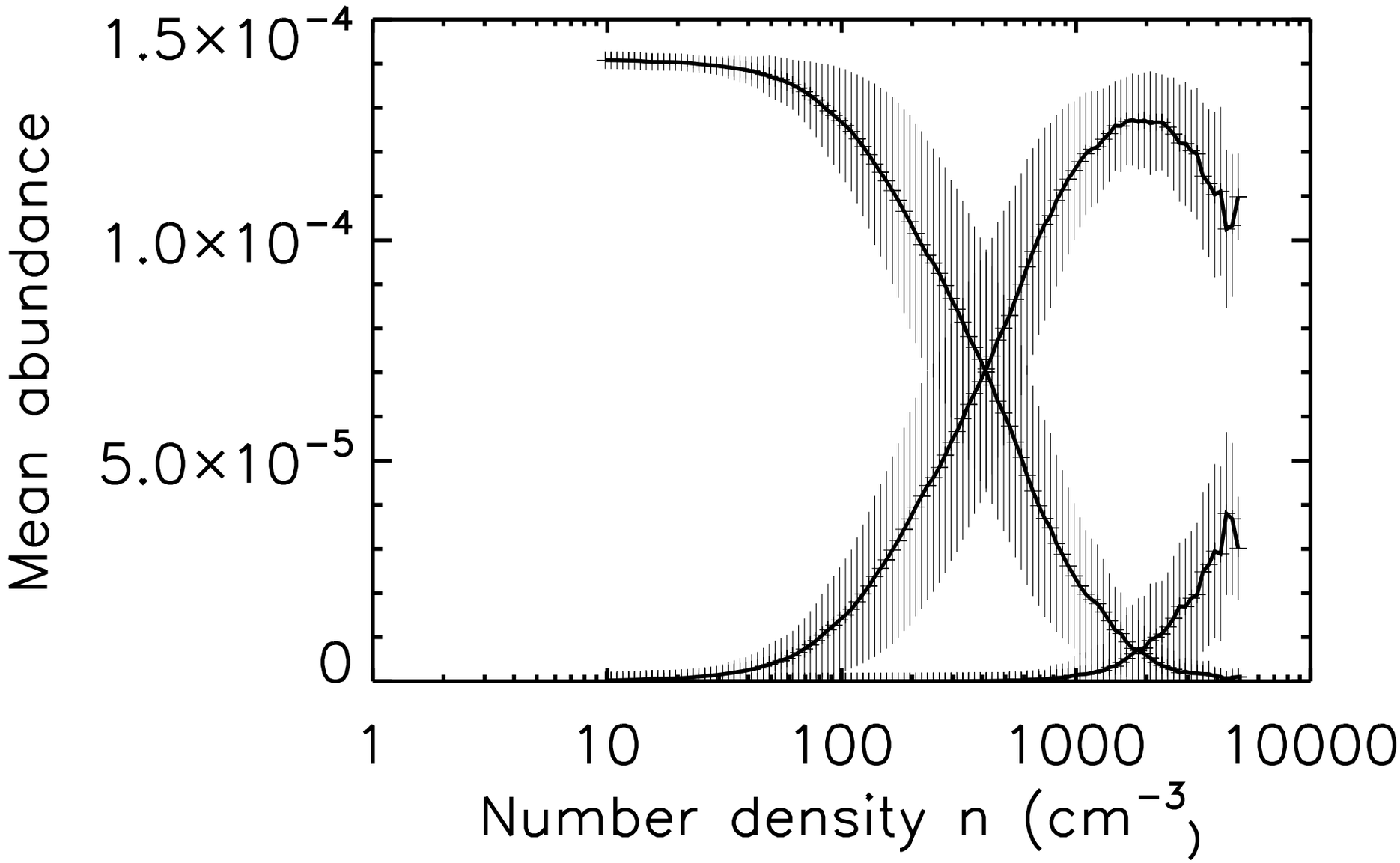
# CO formation

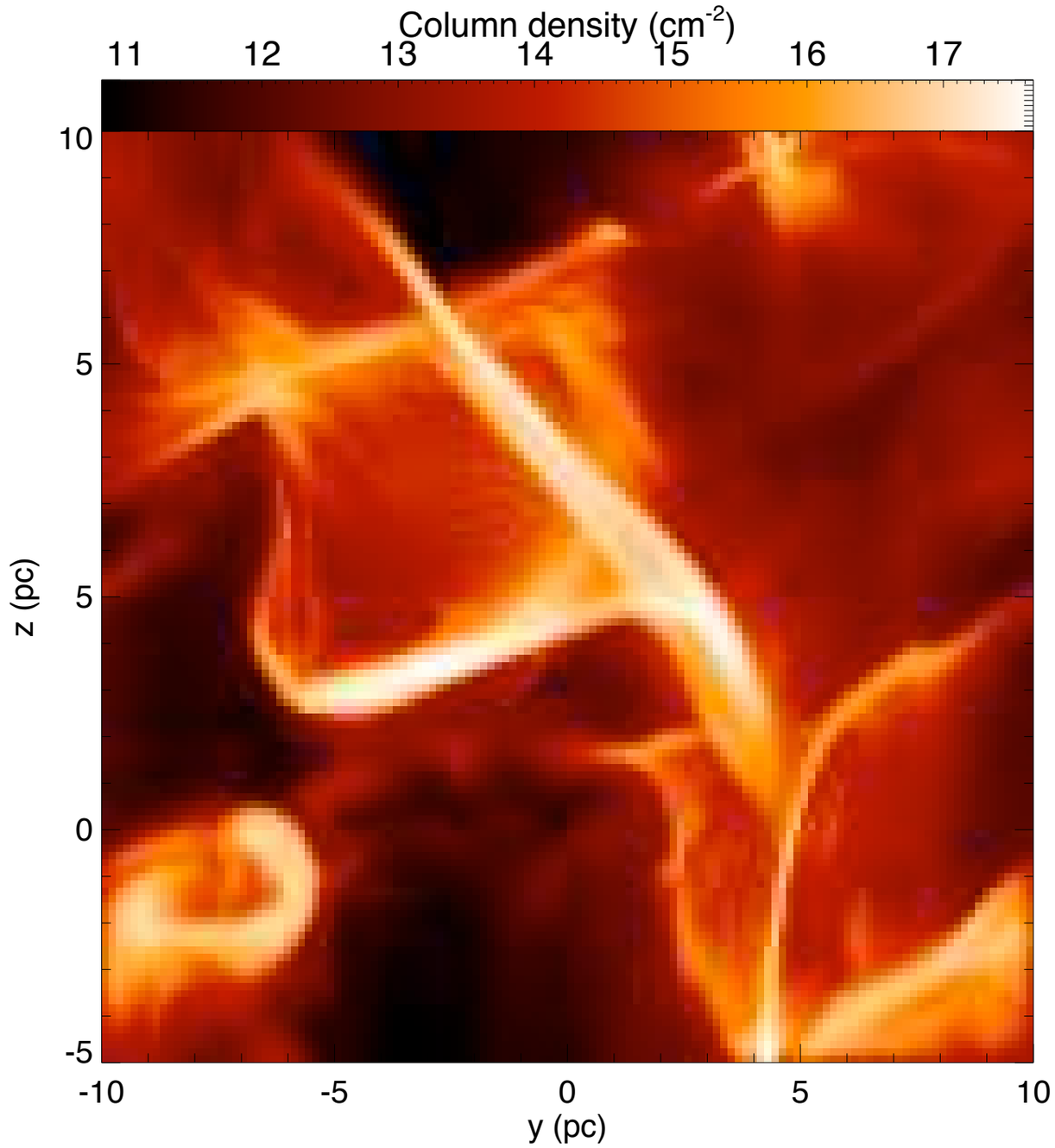
- Same basic approach as $H_2$ formation models

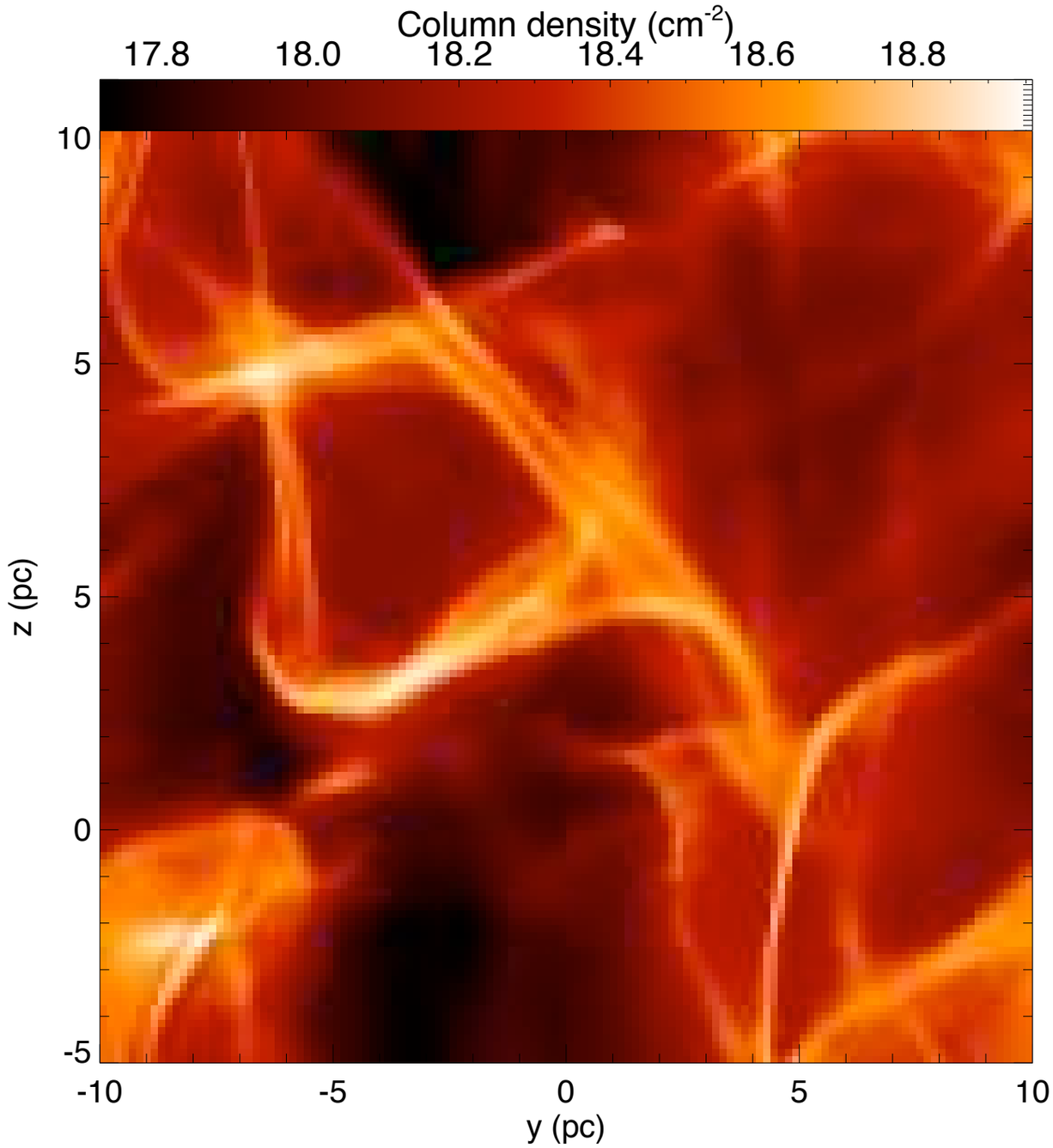
- BUT: chemical network is far more complex...

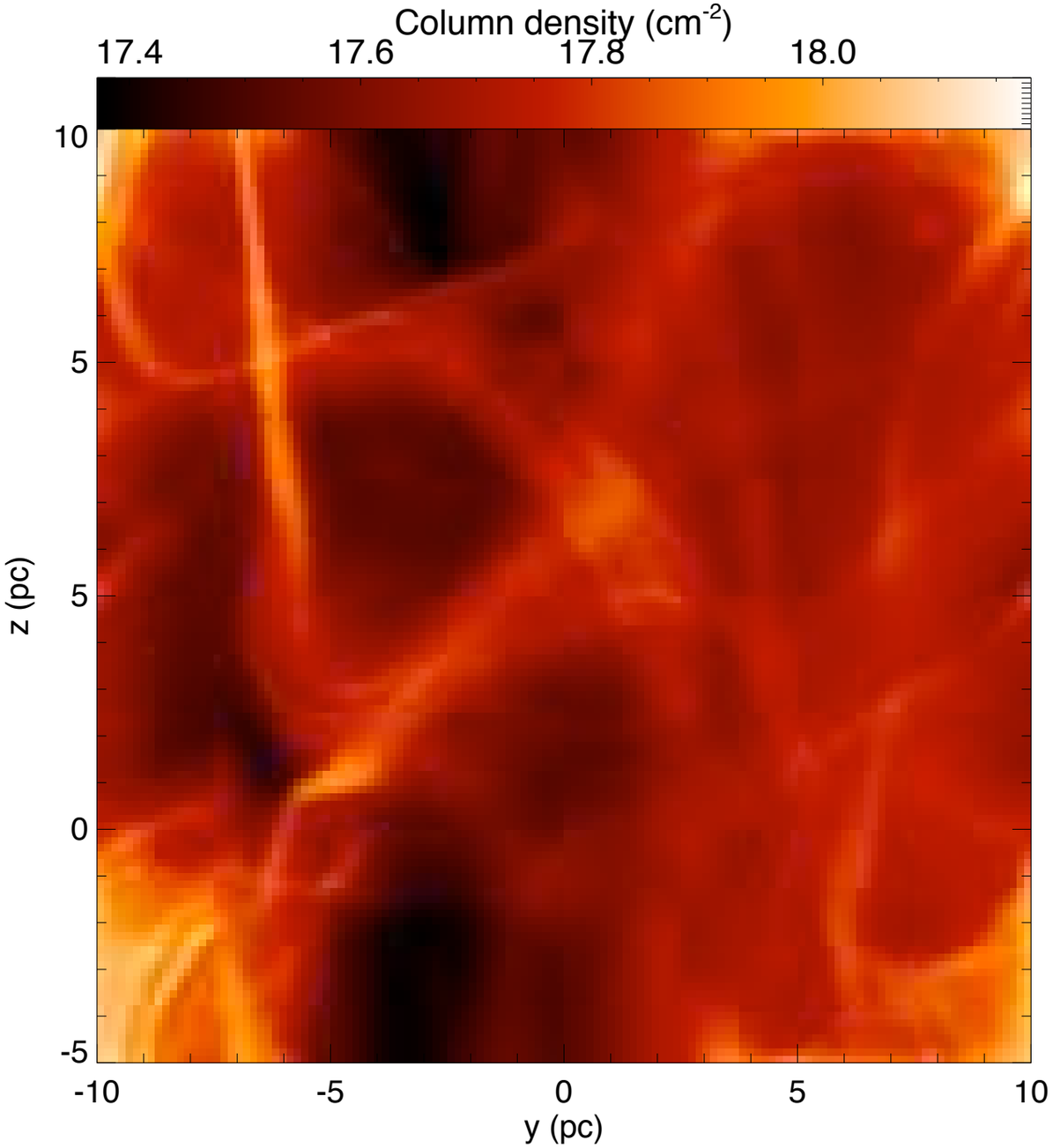
- 18 advected species, 13 equilibrium species, ~ 300 reactions (not including grain surface chemistry)

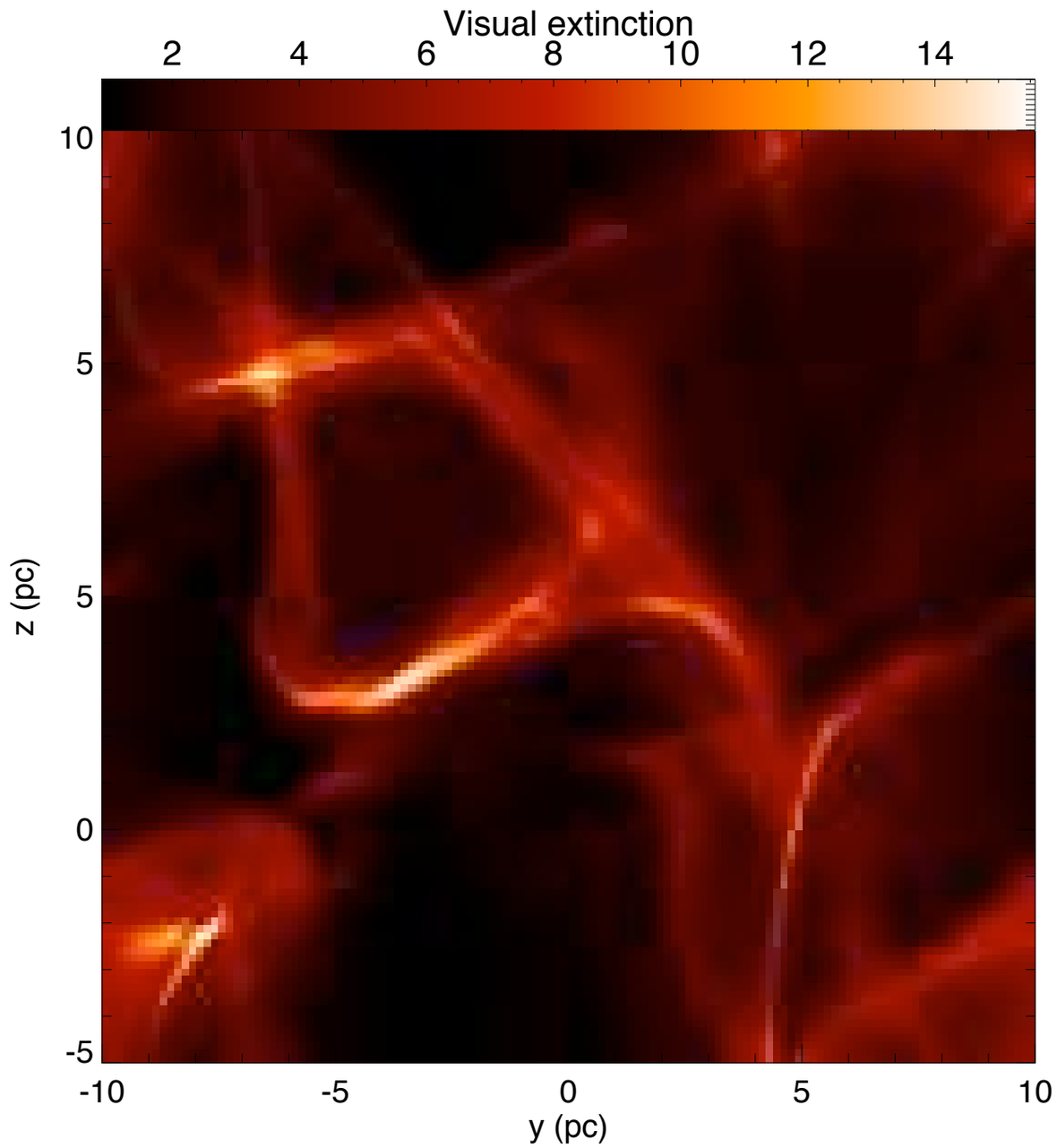

Mass−weighted fractional abundance
$10^{-4}$
$10^{-5}$
$10^{-6}$
$10^{-7}$
$C^+$
C
CO
0
0.5
1
1.5
2
Time (Myr)


1.5×10⁻⁴
1.0×10⁻⁴
5.0×10⁻⁵
0
Mean abundance
V
Λ
1
10
100
1000
10000
Number density n (cm⁻³)


Column density (cm$^{-2}$)
11
12
13
14
15
16
17
10
5
0
-5
z (pc)
-10
-5
0
5
10
y (pc)


Column density (cm$^{-2}$)
17.8
18.0
18.2
18.4
18.6
18.8
10
5
0
-5
z (pc)
-10
-5
0
5
10
y (pc)


Column density (cm-2)
17.4
17.6
17.8
18.0
10
5
0
-5
z (pc)
-10
-5
0
5
10
y (pc)


Visual extinction
2
4
6
8
10
12
14
10
5
0
-5
z (pc)
-10
-5
0
5
10
y (pc)