Can deuteration be used as a chemical clock in protostellar cores

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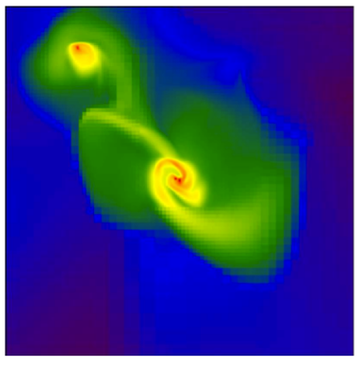
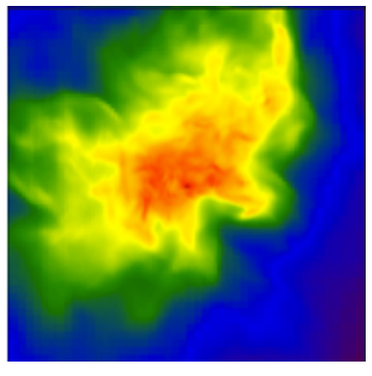
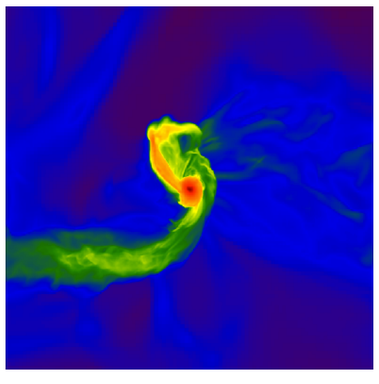
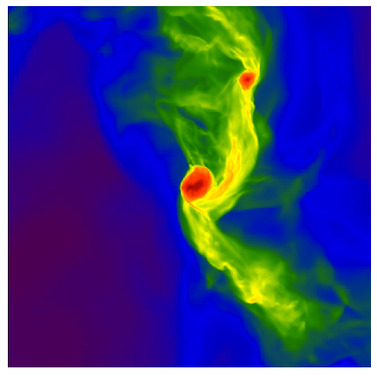

Collaborators:
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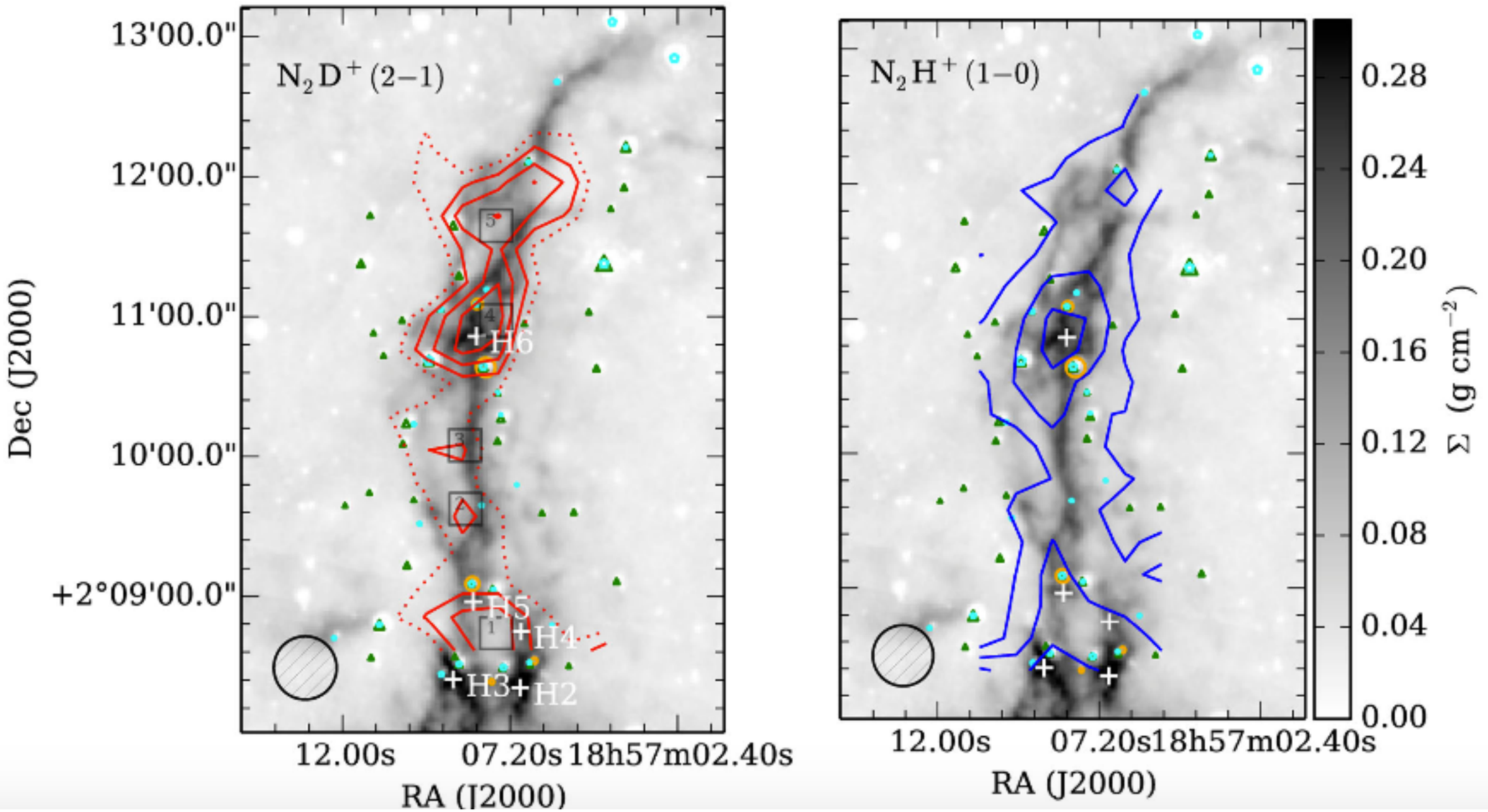
Deuteration in IRDC G035.39−00.33

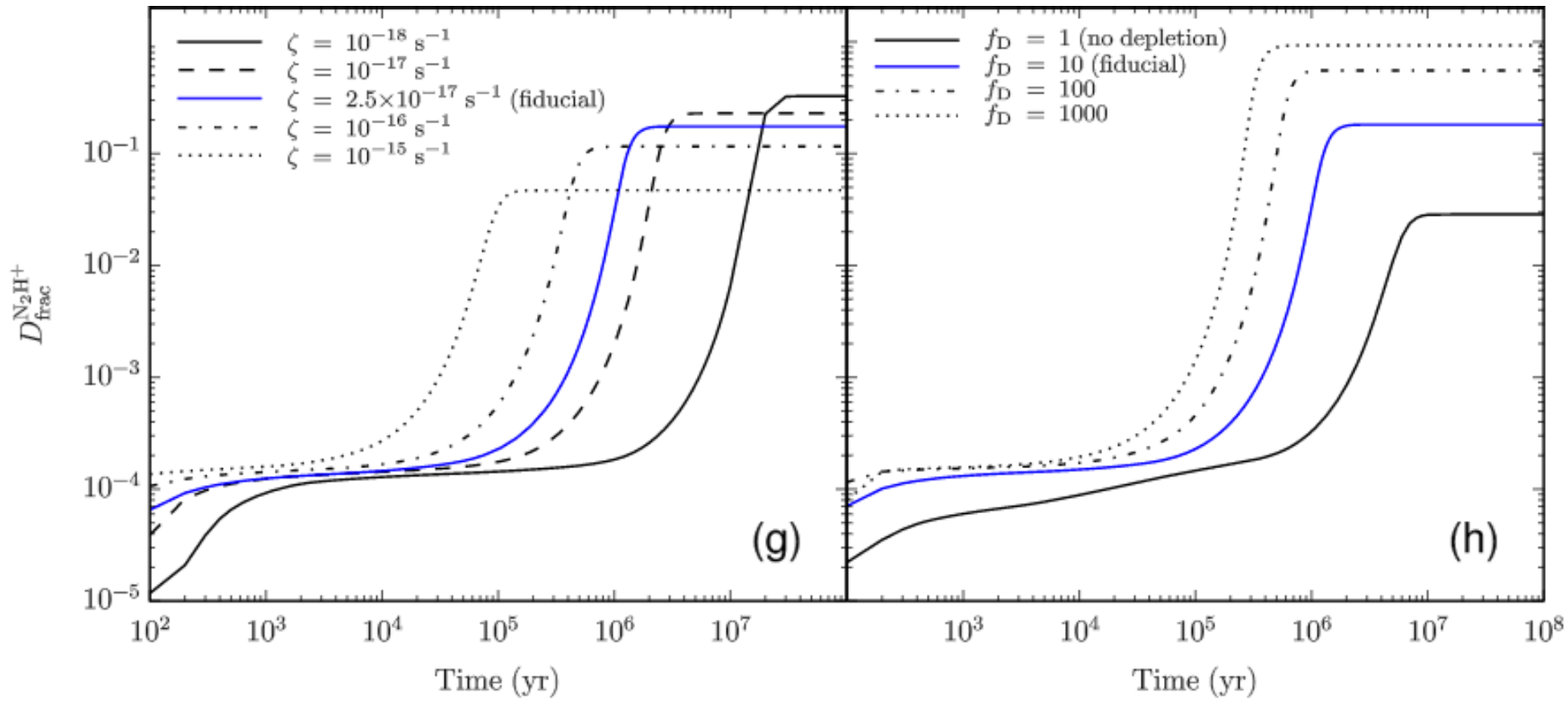


Barnes et al. (2016)

Deuteration of molecules

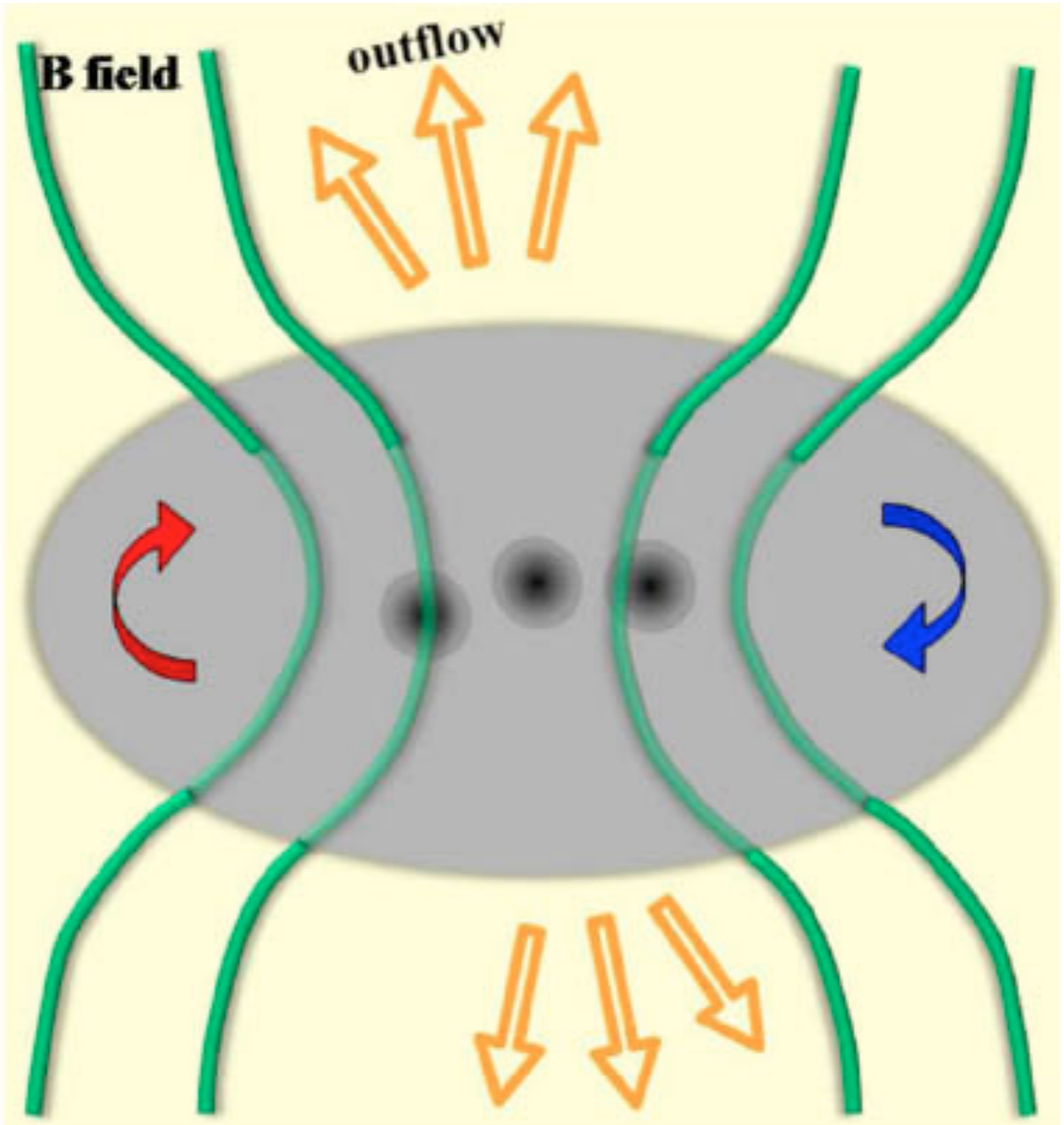
$$H + D^+ \rightarrow H^+ + D,$$
$$H^+ + D \rightarrow H + D^+$$
$$D^+ + H_2 \rightarrow HD + H^+$$

$$H_3^+ + HD \rightarrow H_2D^+ + H_2$$
$$H_2D^+ + HD \rightarrow D_2H^+ + H_2$$
$$D_2H^+ + HD \rightarrow D_3^+ + H_2$$



Kong et al. (2015)

High deuteration fractions: magnetically dominated star formation?



Magnetic field

$$\text{Magnetic flux} = \Phi = B\,A$$

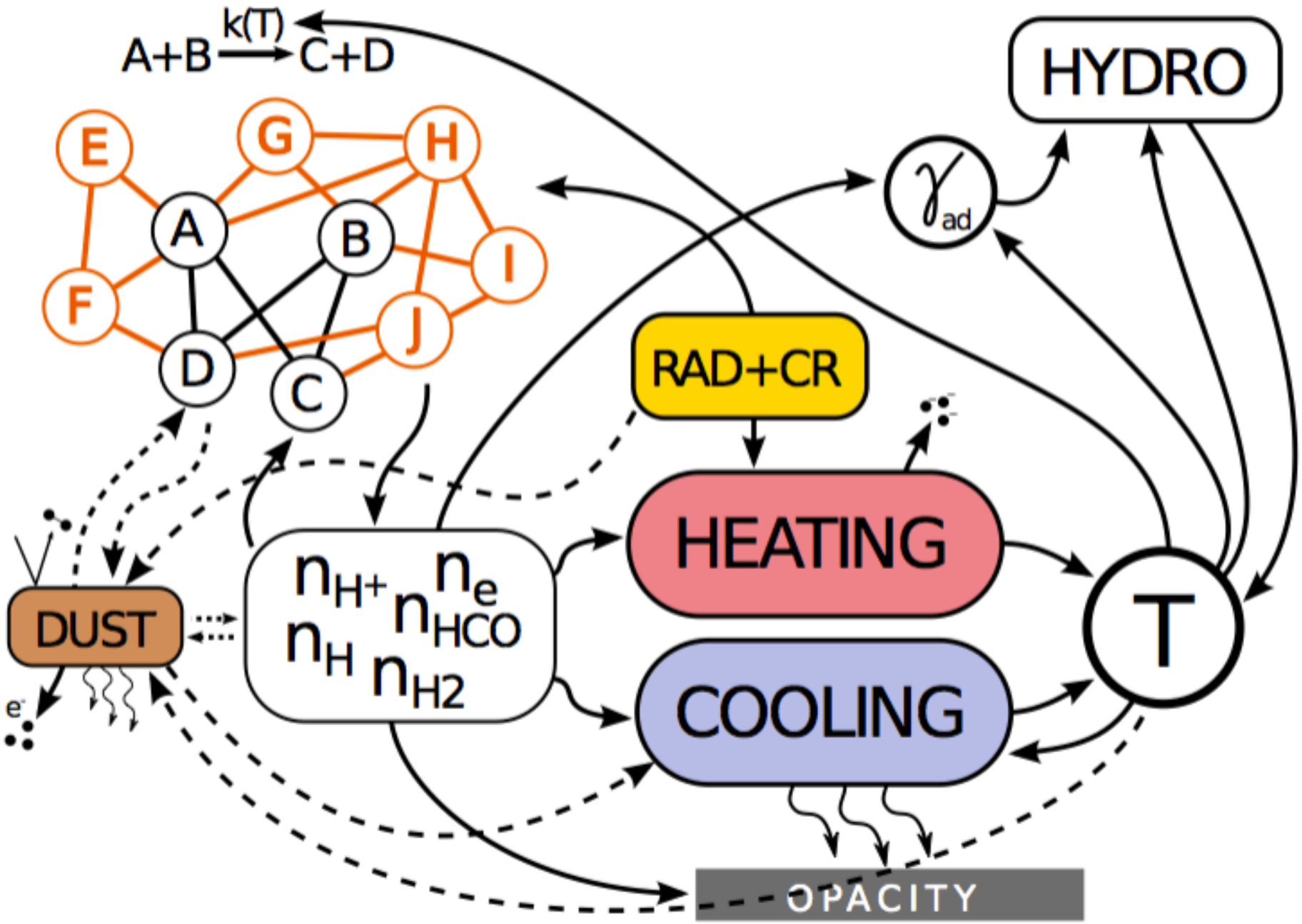
Area perpendicular to magnetic field B

critical mass to collapse:

$$M_J^B = \frac{\Phi}{2\pi\sqrt{G}}$$

magnetic field -> slow collapse -> time for deuteration?

Chemical complexity



Grassi, Bovino, Schleicher et al. (2014)

The chemistry package KROME

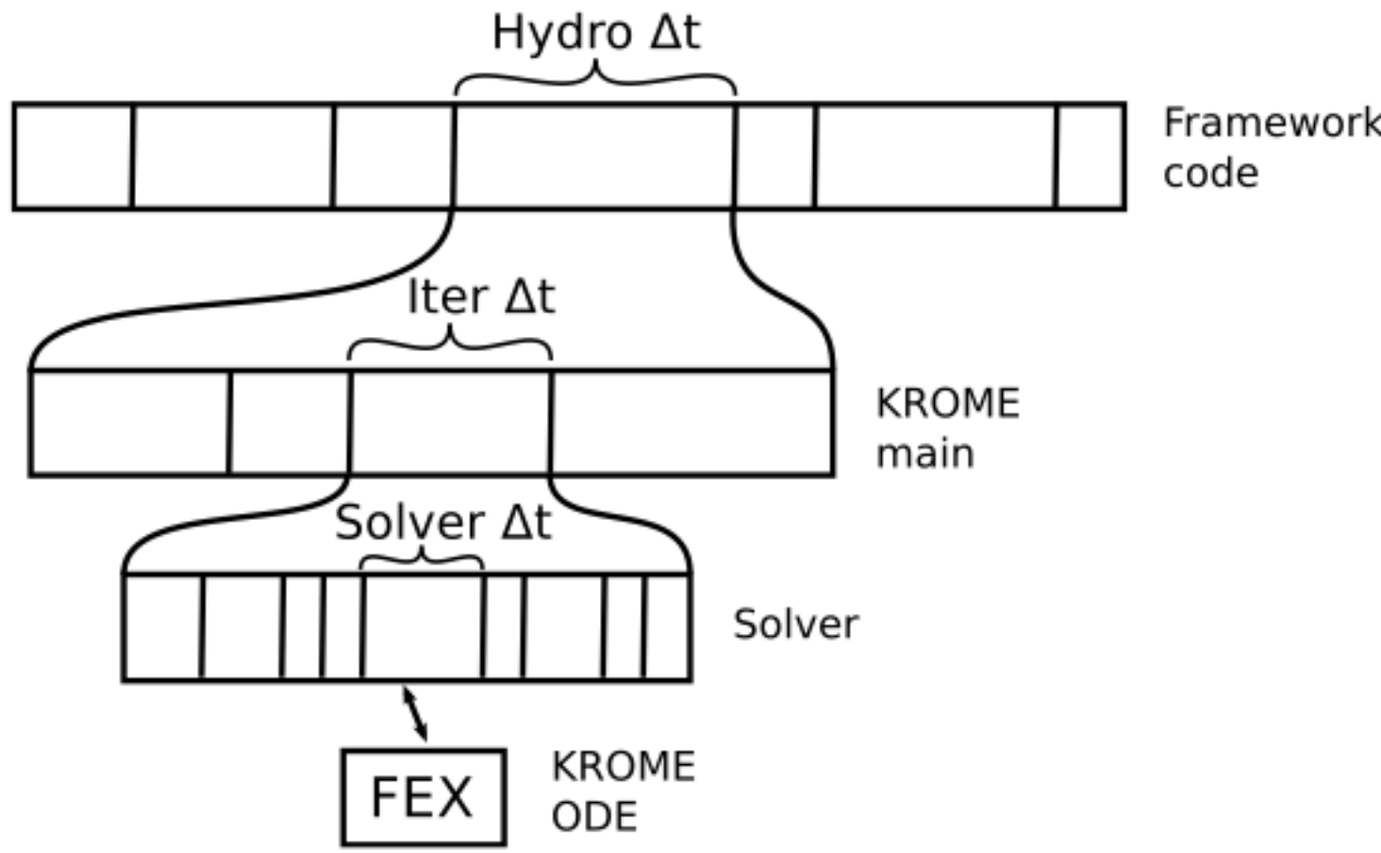
- KROME:
  phython module to create Fortran subroutine
  for existing chemical networks.

- The subroutine is then included in the framework code.

- Existing interfaces for Enzo, Flash, Gasoline, Ramses
  (plus wrapper for C++).

- Several example networks
  as well as user-defined
  networks.

- Publicly available:
  www.kromepackage.org



Grassi, Bovino, Schleicher et al. (2014)

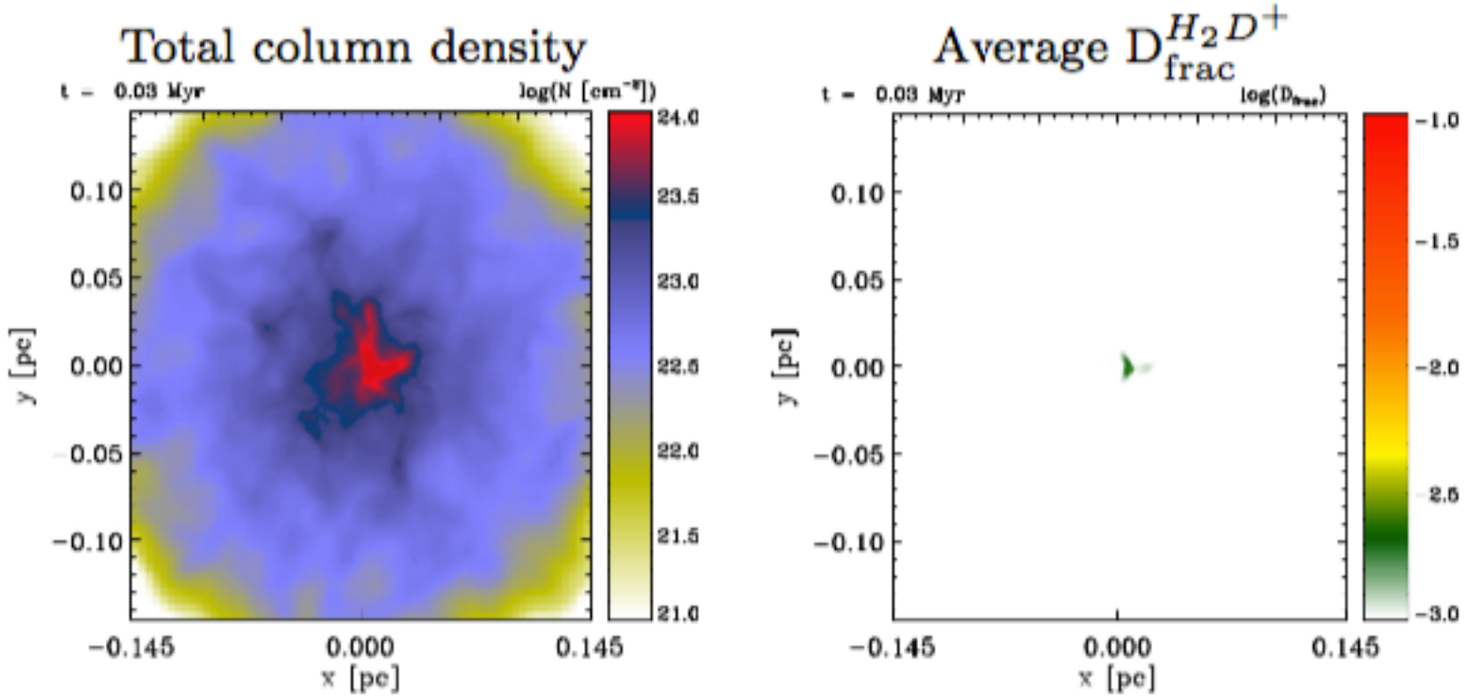
Test with 3D numerical simulations

- 60 solar mass core, 0.17 pc, 15 K,
  turbulent Mach number of 2
- mass to flux ratio: ~10 above critical value
- maximum resolution: 235 AU
- magneto-hydrodynamics + self-gravity
  solved with the FLASH code
- network for deuteration chemistry based on
  Walmsley et al. (2004)

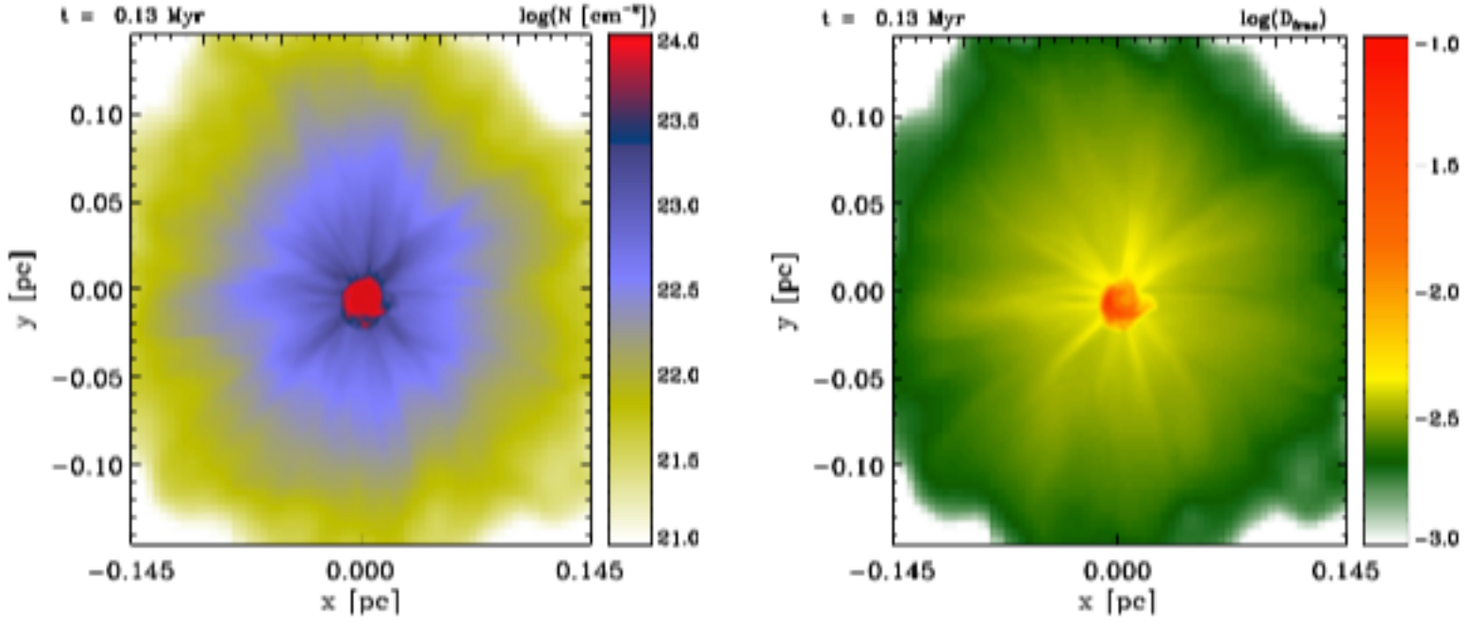
Koertgen, Bovino, Schleicher et al., submitted
(arXiv:1703.01201)

Results reference run

30 kyrs:



130 kyrs:



Koertgen, Bovino, Schleicher et al., submitted
(arXiv:1703.01201)

Total number of simulations

Surface density $\left(\mathrm{g/cm^2}\right)$	Core radius (pc)	Core mass ($\mathrm{M_\odot}$)	Av. Field strength (μG)	Mass–to–flux ratio[a] μ/μ_{crit}	Mach number $\mathcal{M}_{\mathrm{turb}}$	Virial parameter α_{vir}
0.14	0.17	60	27	10	1	0.16
0.14	0.17	60	27	10	2	0.64
0.14	0.17	60	27	10	2	0.64
0.14	0.17	60	27	10	2	0.64
0.14	0.17	60	27	10	2	0.64
0.14	0.17	60	27	10	4	2.56
0.14	0.17	60	27	10	6	5.76
0.14	0.17	60	27	10	12	23.04
0.14	0.17	60	54	5	2	0.64
0.14	0.17	60	54	5	4	2.56
0.14	0.17	60	108	2.5	0.5	0.04
0.14	0.17	60	108	2.5	2	0.64
0.14	0.17	60	108	2.5	6	5.76
0.24	0.08	27	49	10	2	0.71
0.24	0.08	27	98	5	2	0.71
0.39	0.1	60	76	10	0.5	0.03
0.39	0.1	60	76	10	2	0.48
0.39	0.1	60	76	10	2	0.48
0.39	0.1	60	152	5	2	0.48
0.39	0.1	60	304	2.5	2	0.48
0.39	0.1	60	304	2.5	4	1.92

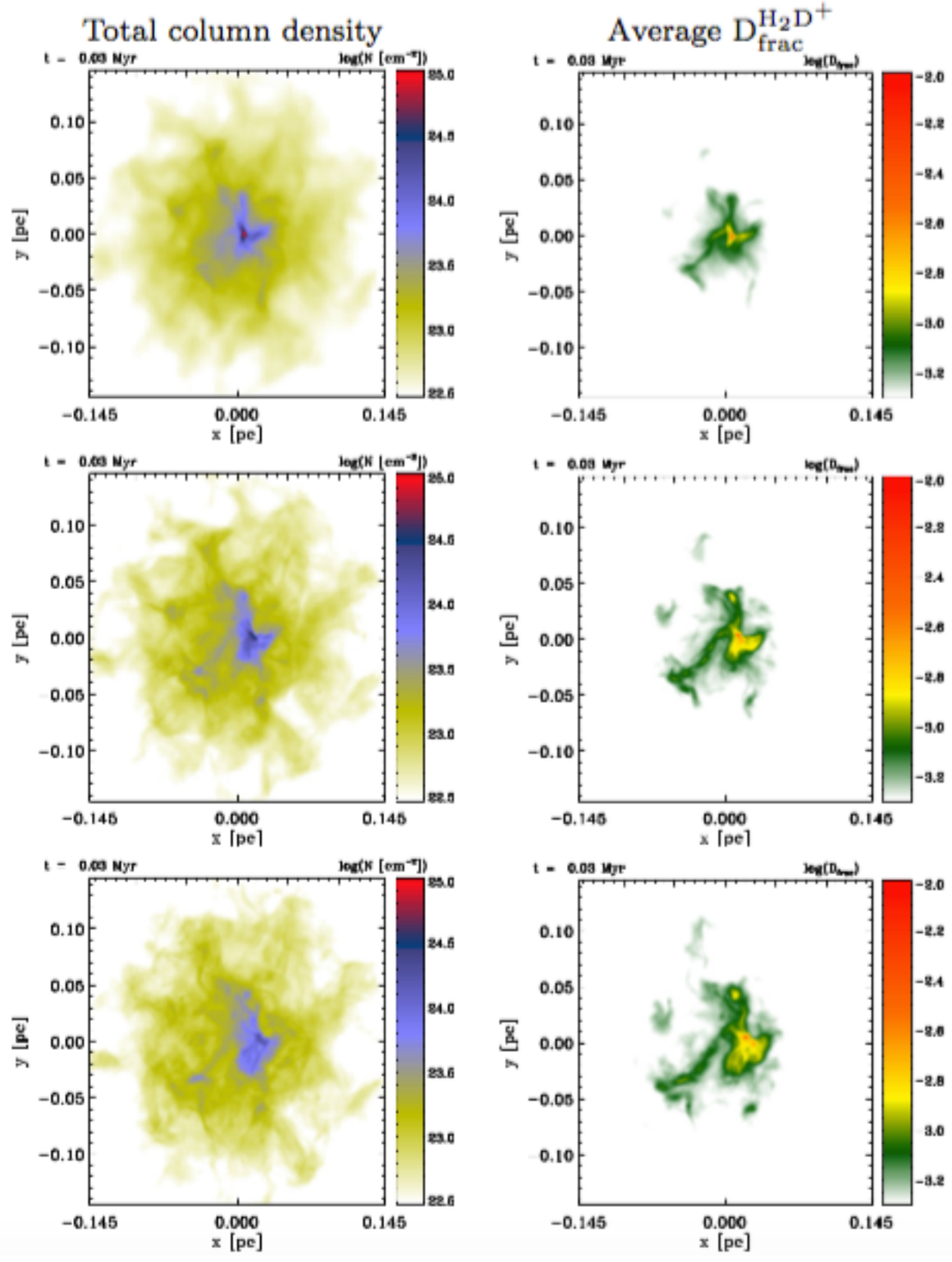
Koertgen, Bovino, Schleicher et al., submitted
(arXiv:1703.01201)

Dependence on turbulent Mach number

M=2

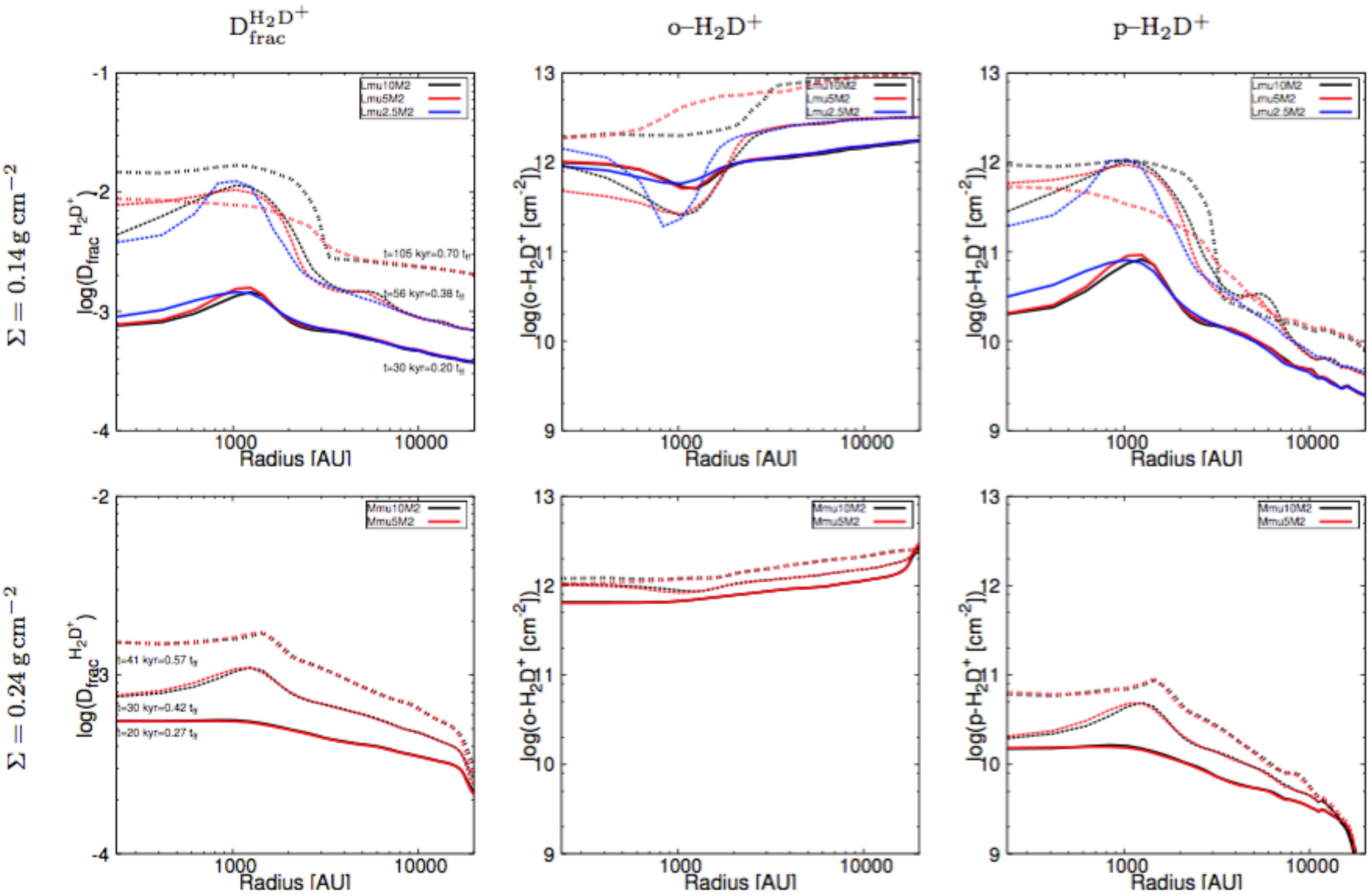
M=4

M=6



Koertgen et al., submitted

Dependence on mass-to-flux ratio



Koertgen, Bovino, Schleicher et al., submitted
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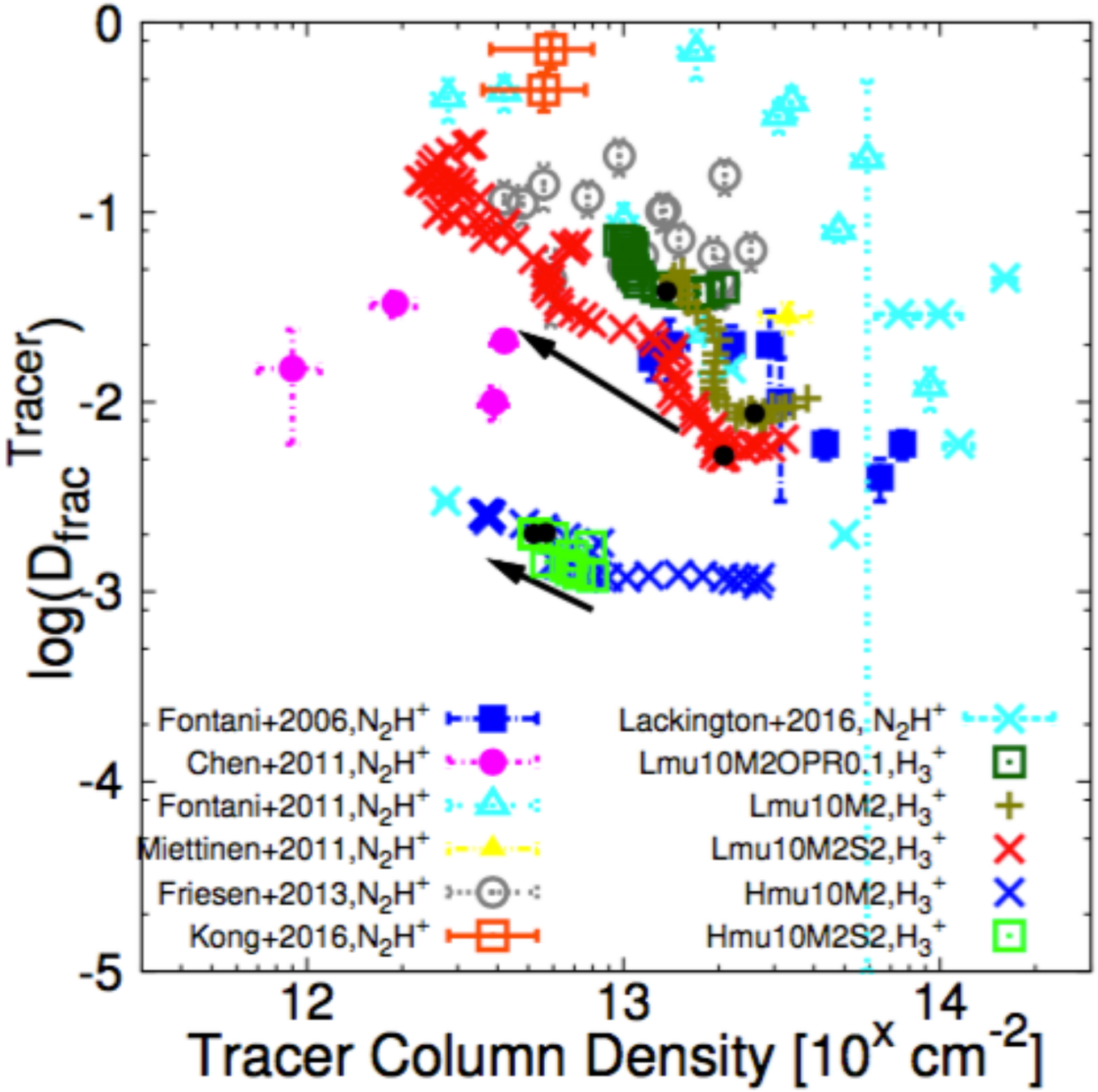
Comparison with observational data



Koertgen, Bovino, Schleicher et al., submitted
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Summary

- Observed deuteration fraction can be readily reproduced in numerical simulations.
- The deuteration fraction is roughly independent of the magnetic field, and depends weakly on the initial surface density and turbulent Mach number.
- Important to explore chemical uncertainties like incomplete depletion both with high-resolution observations as well as chemical investigations.
- Need to better understand the initial conditions:
  What is the ortho-to-para ratio on large scales? How good is the approximation of high depletion?