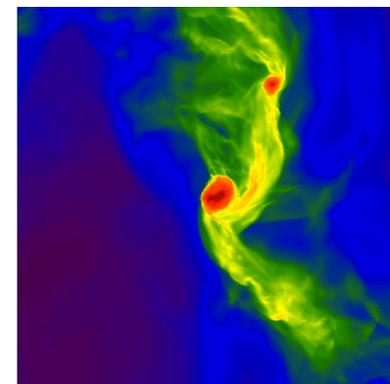
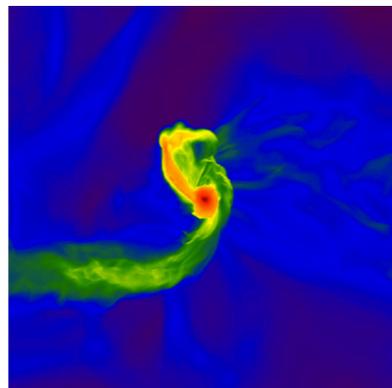
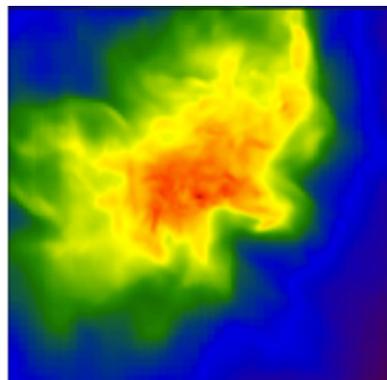
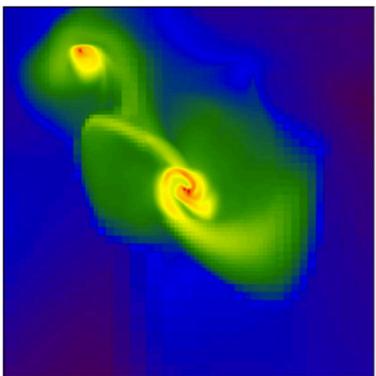




Introduction to Computational Astrochemistry

Dominik Schleicher
Departamento de Astronomía
Universidad de Concepción



Collaborators:

Robi Banerjee (Hamburg), Stefano Bovino (Hamburg), Pedro Capelo (Zürich), Stephanie Dörschner (Göttingen), Andrea Ferrara (Pisa), Daniele Galli (Florence), Tommaso Grassi (Copenhagen), Troels Haugboelle (Copenhagen), Muhammad Latif (Paris), Jens Niemeyer (Göttingen), Francesco Palla (Florence), Wolfram Schmidt (Hamburg), Marco Spaans (Groningen), Caroline Van Borm (Groningen)

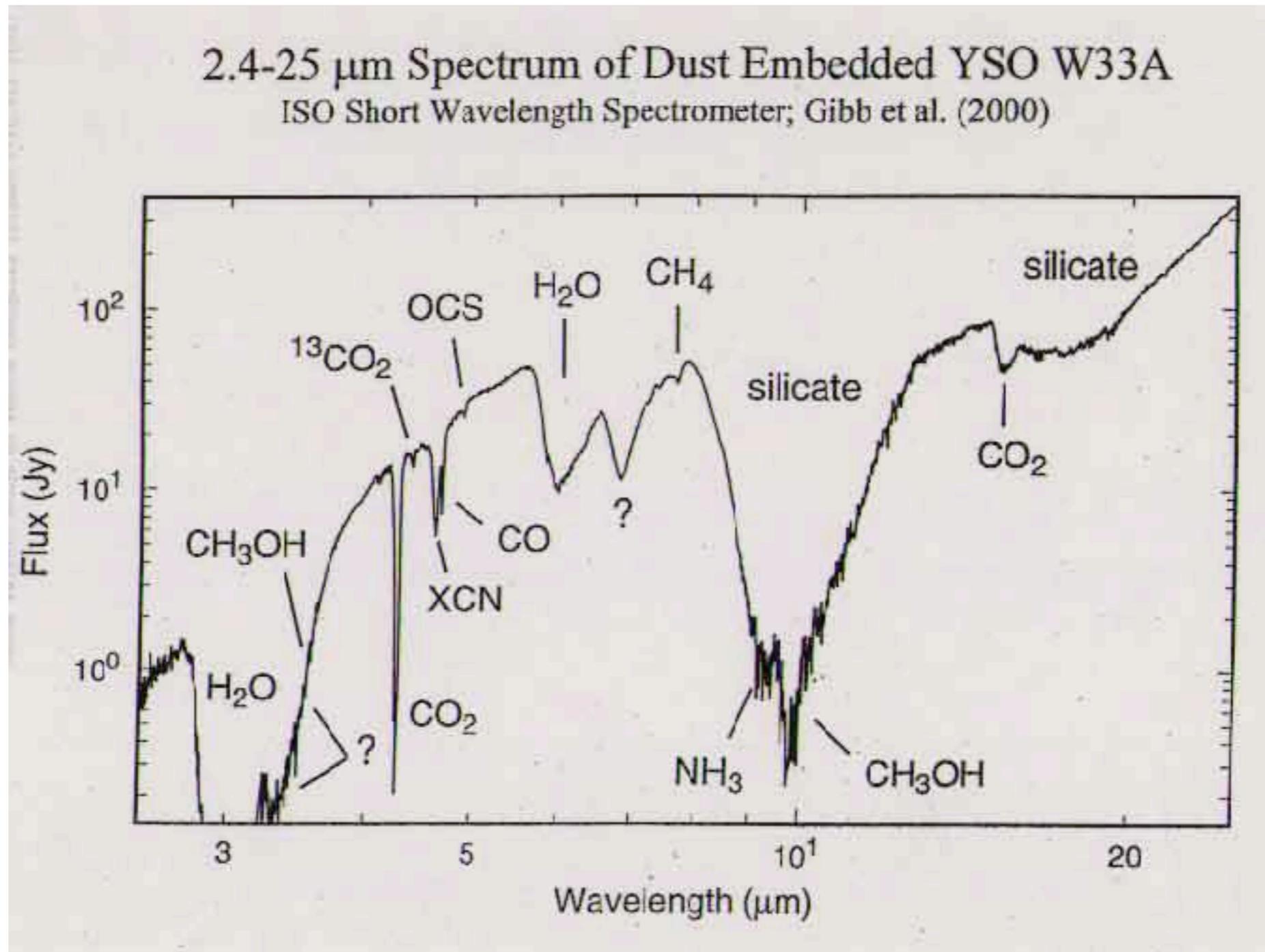
Contents

- Motivation: Why chemistry in simulations?
- Implementation / general issues
- KROME: A short overview
- Some applications

Motivation: Why chemistry?

- Modeling:
 - Chemistry and cooling determines the **equation of state**.
 - The equation of state of the gas regulates gravitational instabilities and **fragmentation**.
- Comparison with observations:
 - Astrophysical objects are often observed through the **line emission of different atoms, ions or molecules**.
 - A comparison with hydrodynamical simulations requires to include these species in the **chemical modeling**.

Motivation: Line emission in young stellar objects



Gibb et al. (2000)

I D structure of photodissociating regions

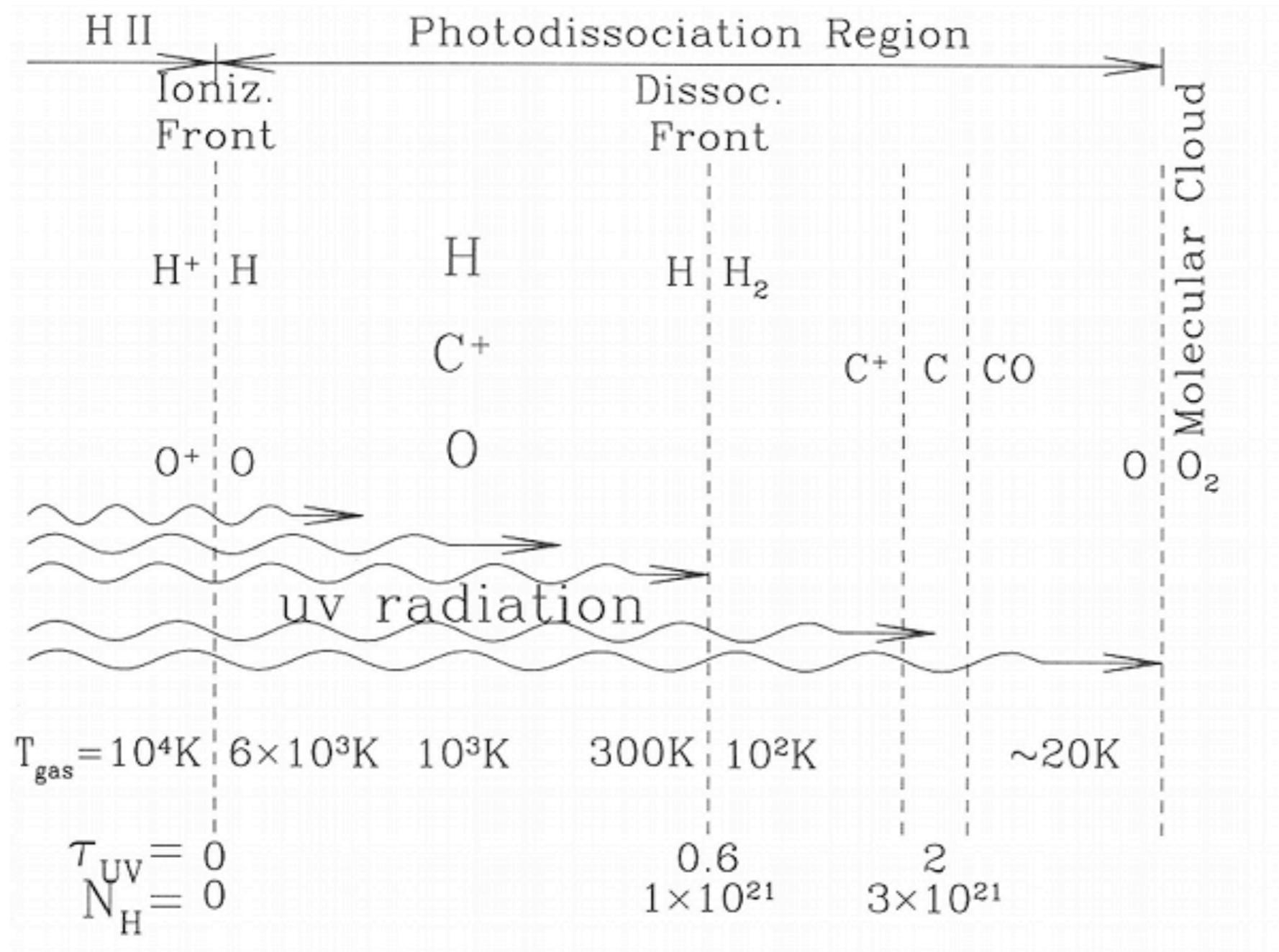
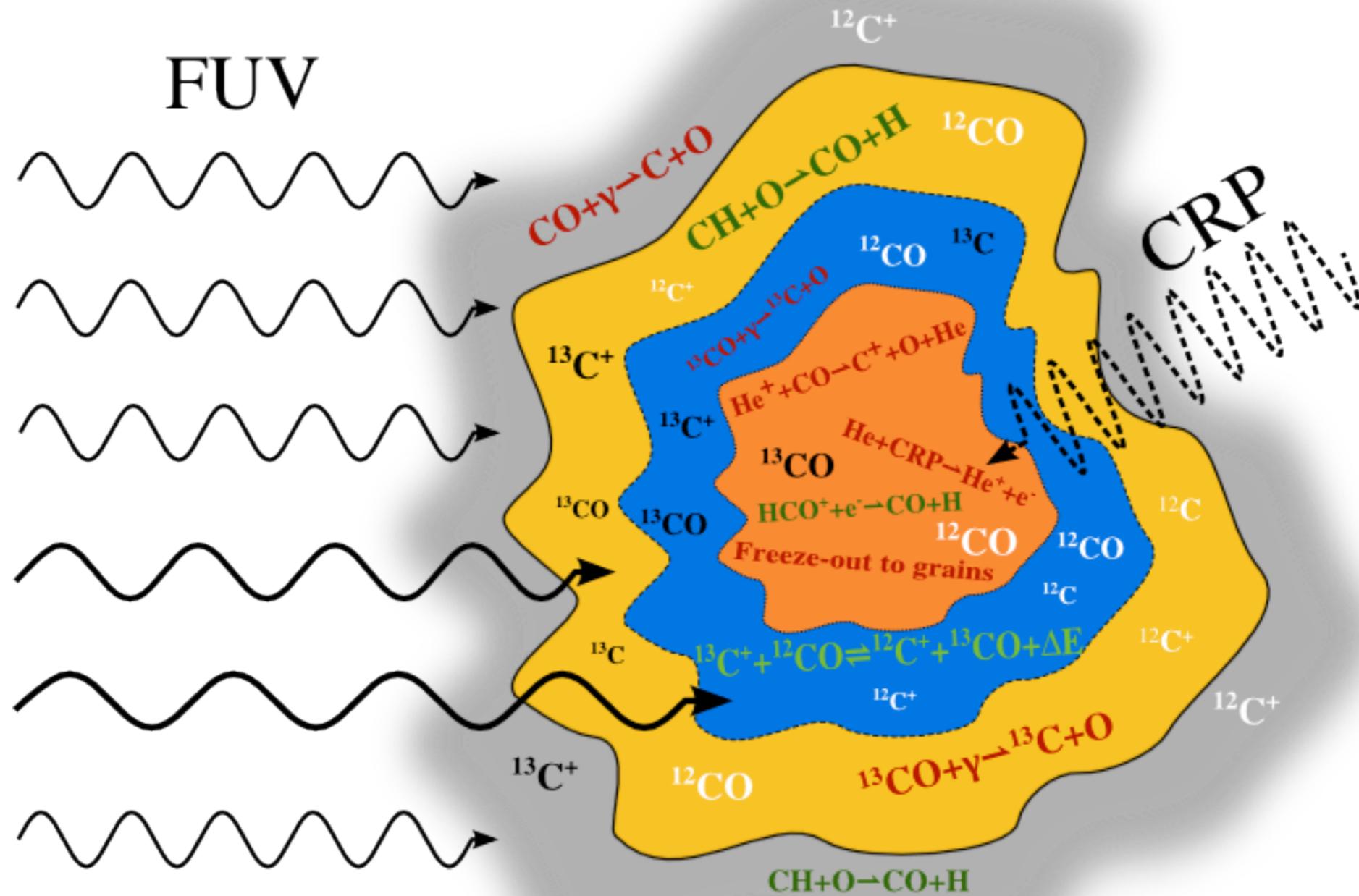


Figure 31.2 Structure of a PDR at the interface between an H II region and a dense molecular cloud.

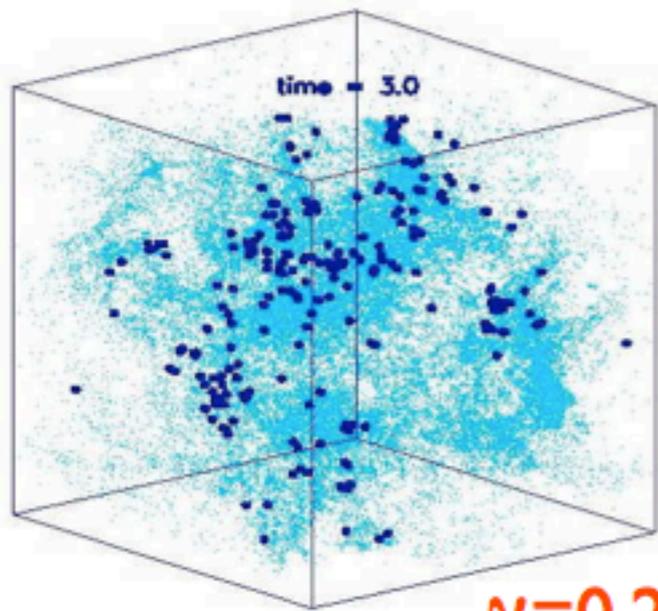
Bruce Draine (2011)

3D structure of turbulent molecular clouds

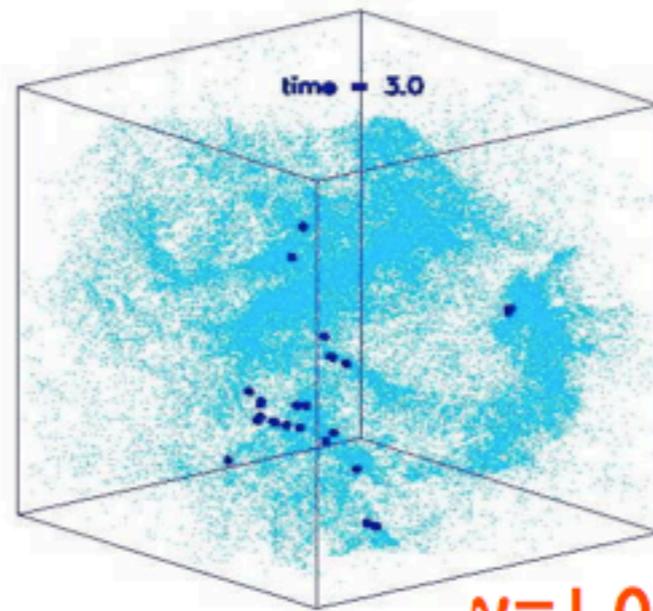


Szücs et al. (2014)

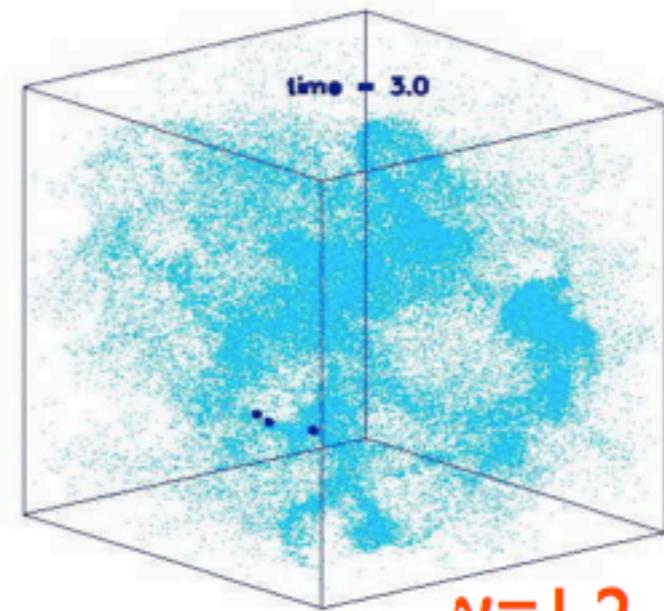
Modeling: Fragmentation and the equation of state



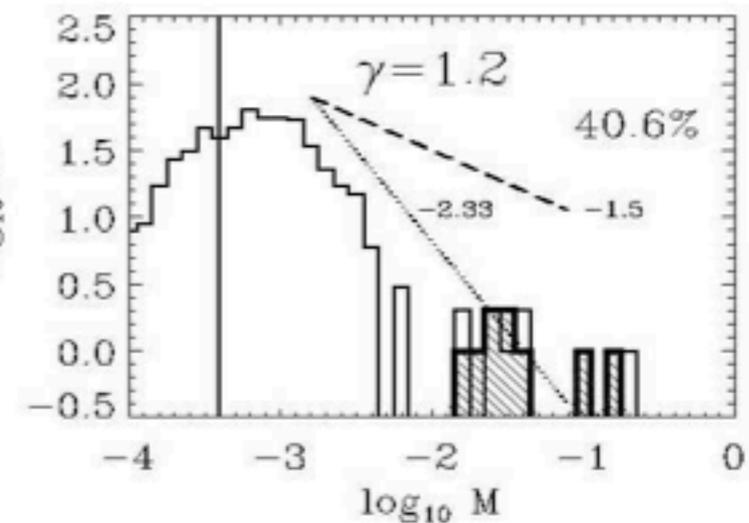
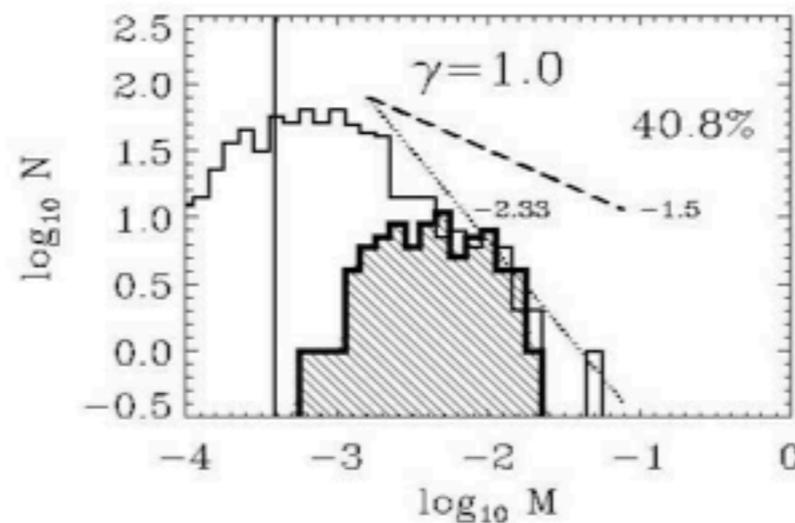
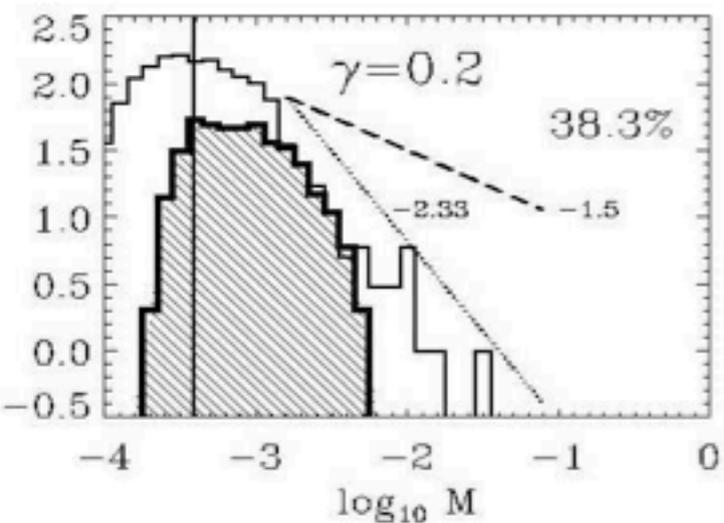
$\gamma=0.2$



$\gamma=1.0$



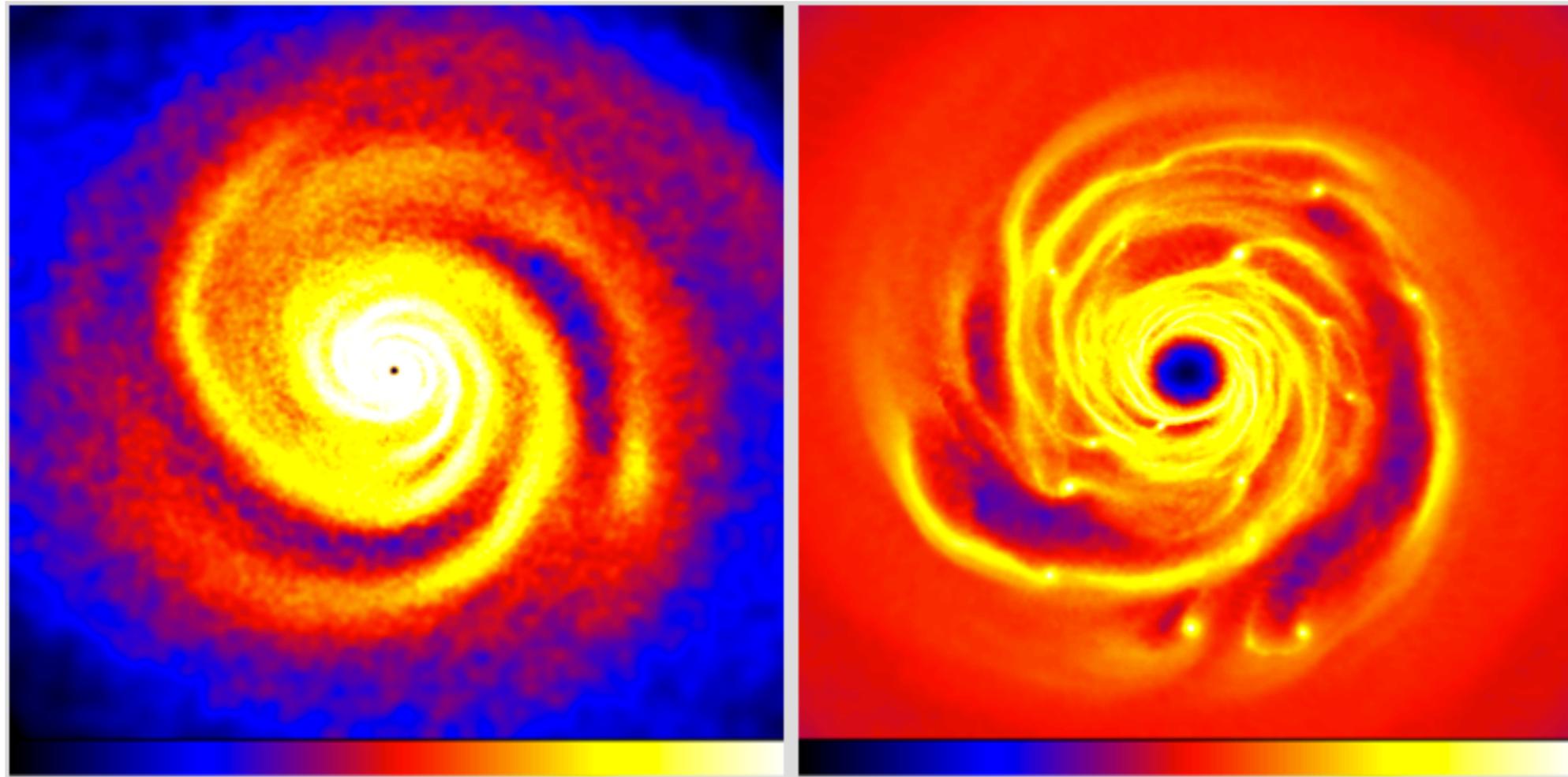
$\gamma=1.2$



Li et al. (2003)

$$\gamma_{eff} = 1 + \frac{d \log T}{d \log \rho}$$

Evolution of self-gravitating disks



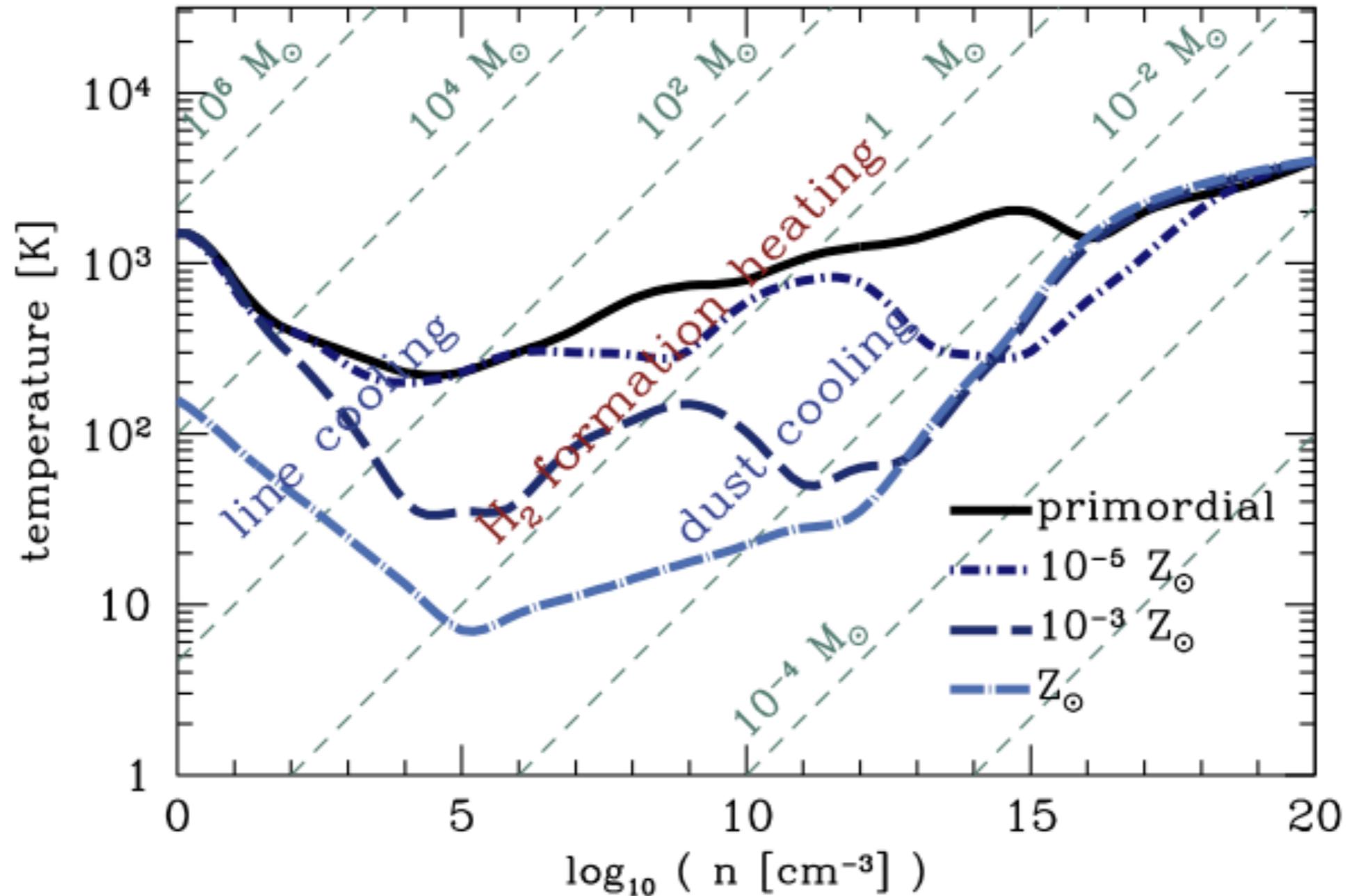
long cooling time

short cooling time

Rice et al. (2003)

Realistic cooling timescales require chemical modeling!

Thermal evolution for different densities and metallicities



Omukai et al. (2005)

Gas dynamics in 3D simulations

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

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) + \nabla P = \rho \mathbf{g} \quad \text{Euler}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + P) \mathbf{v}] = \rho \mathbf{v} \cdot \mathbf{g} \quad \text{total energy}$$

$$\frac{\partial \rho \epsilon}{\partial t} + \nabla \cdot [(\rho \epsilon + P) \mathbf{v}] - \mathbf{v} \cdot \nabla P = \Lambda \quad \text{internal energy}$$

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

see e.g. FLASH documentionn

Chemistry and cooling

Ideal gas: $\rho\epsilon = \frac{p}{\gamma - 1} = \frac{\rho k T}{(\gamma - 1)\mu}$

Need to determine heating and cooling term.

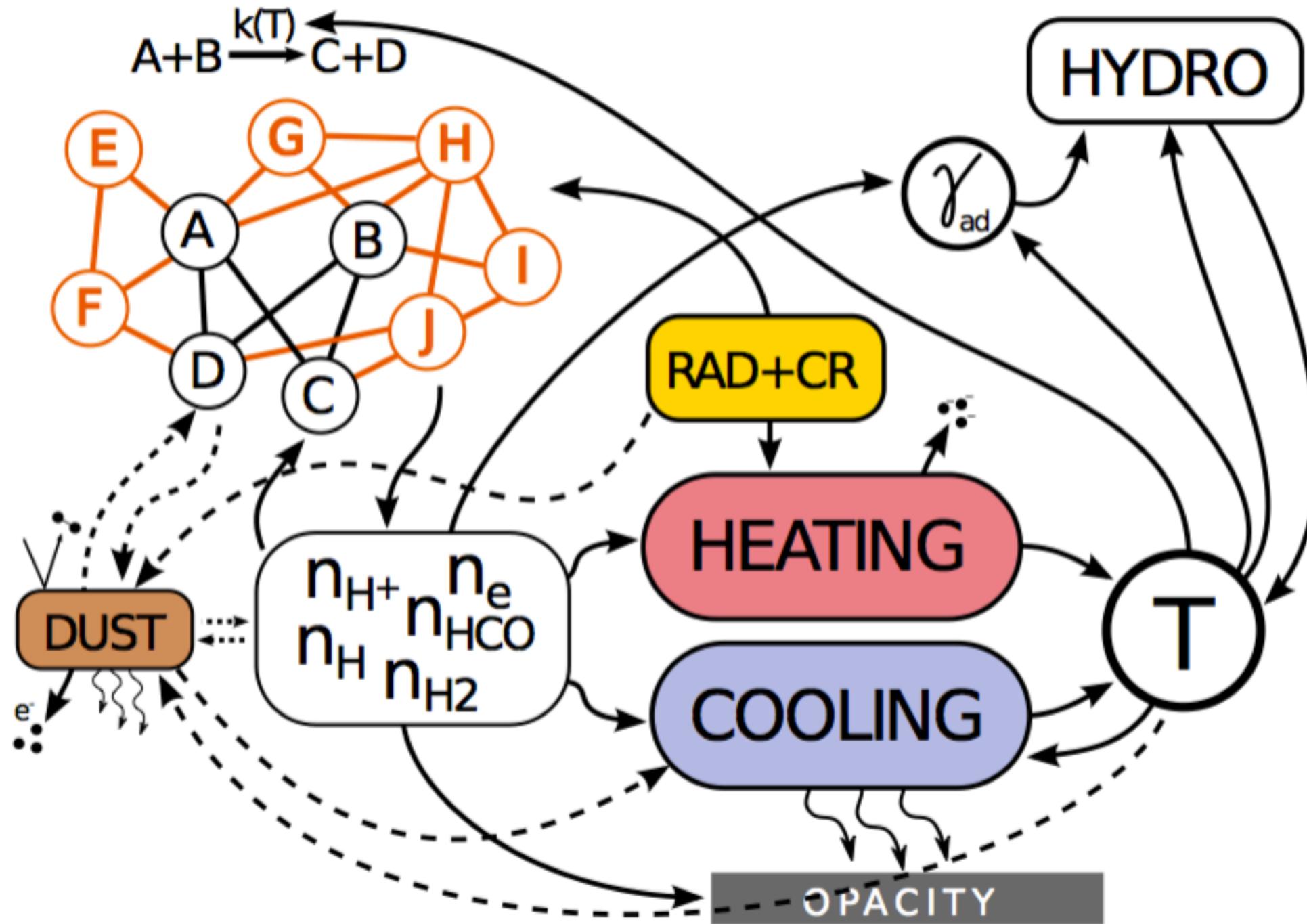
Dependence on temperature and chemical composition!

Rate equations: $\frac{\partial n_i^Z}{\partial t} + \nabla \cdot n_i^Z \mathbf{v} = R_i^Z \quad (i = 1, \dots, N_{spec})$

fluid advection:
treated by hydro

chemical reactions:
KROME: high-order solver DLSODES

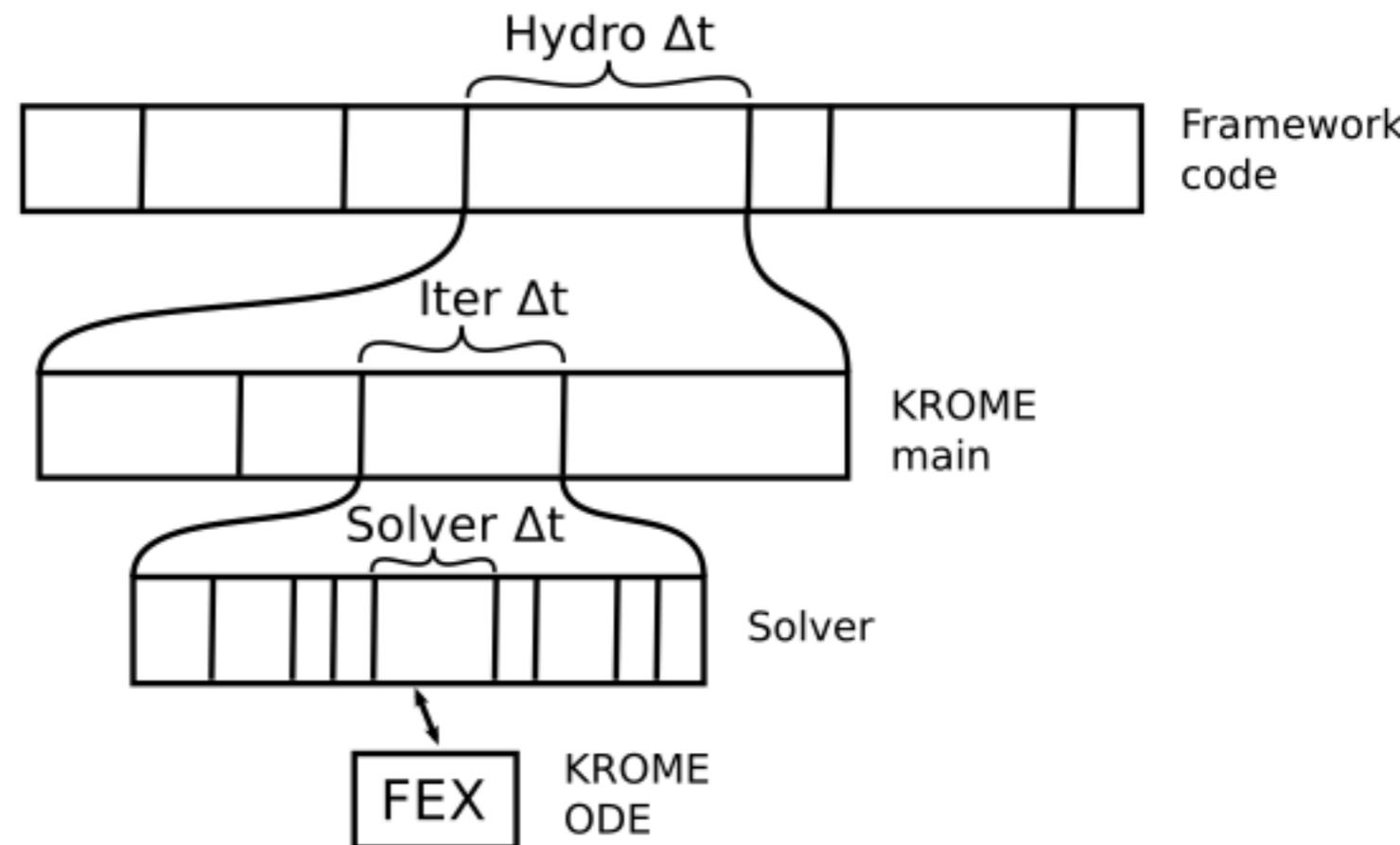
Combining chemistry & cooling with hydrodynamics



Grassi, Bovino, Schleicher et al. (2014)

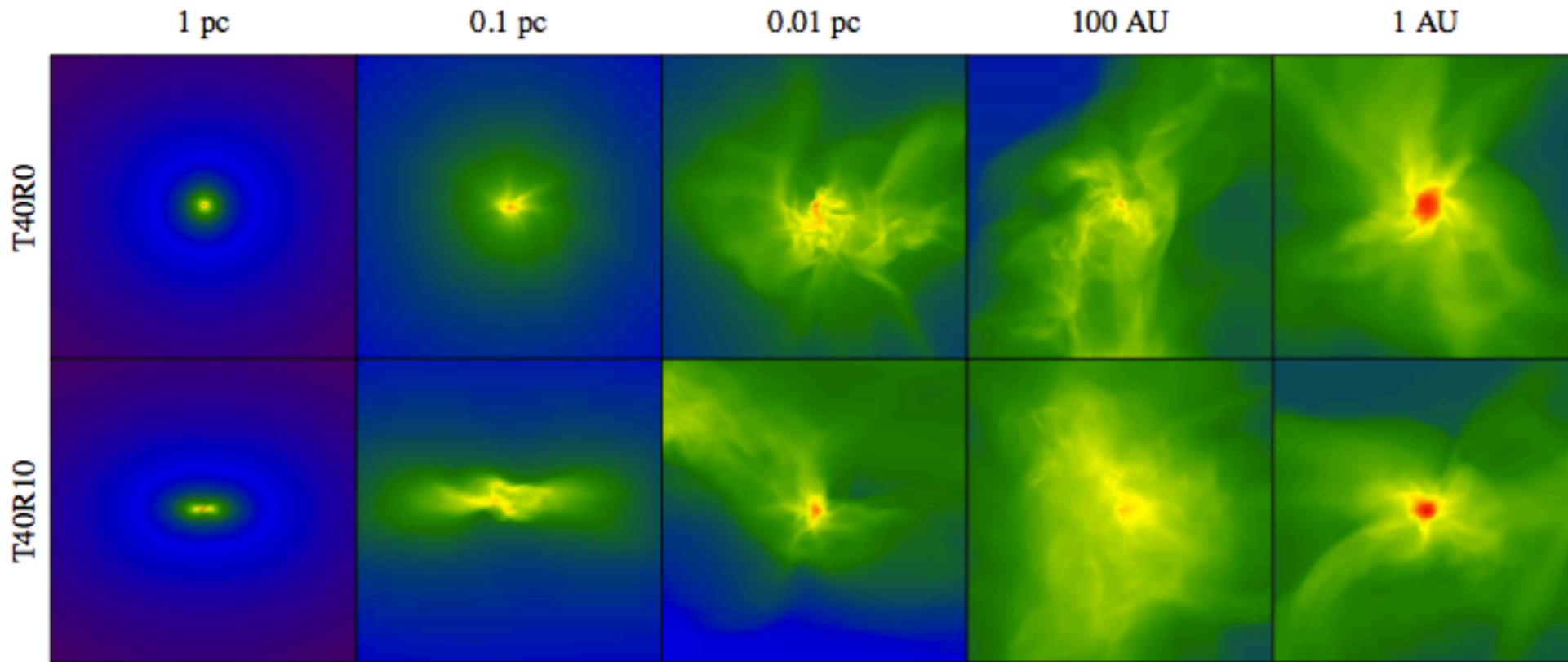
The chemistry package KROME

- KROME:
python 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)

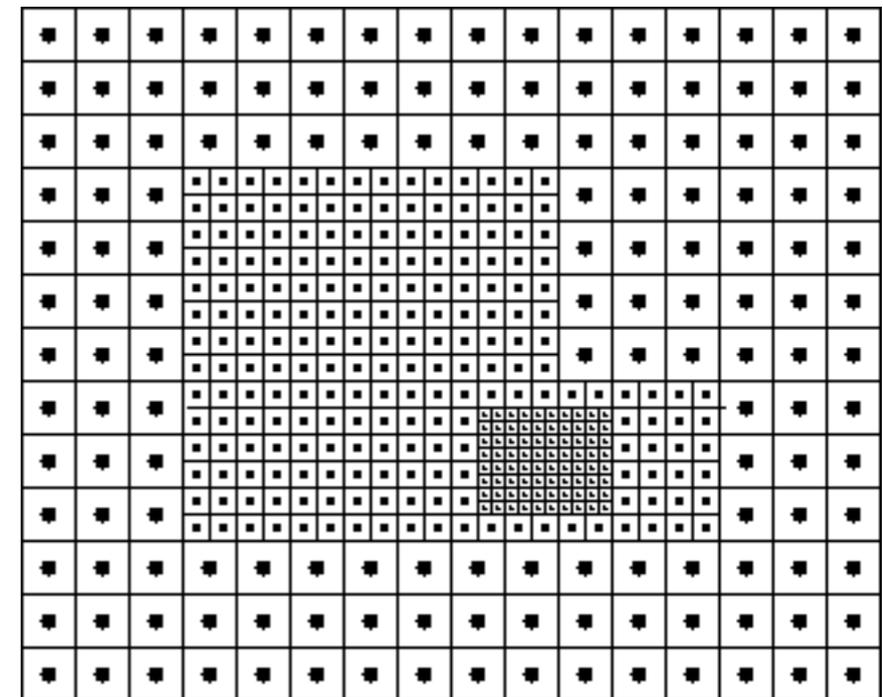
Example: Applications with Enzo



Van Borm et al.
(2014)

3D AMR simulations with Enzo:

- (Magneto-)hydrodynamics
- Gravity
- Chemistry, cooling
- Dark matter



Non-equilibrium chemistry during collapse

Recombination
timescale:

$$t_{rec} = \frac{n_e}{kn_e n_p} \sim \frac{1}{kX_H n_b}$$

Free-fall
timescale:

$$t_{dyn} \sim \frac{1}{\sqrt{G\rho}}$$

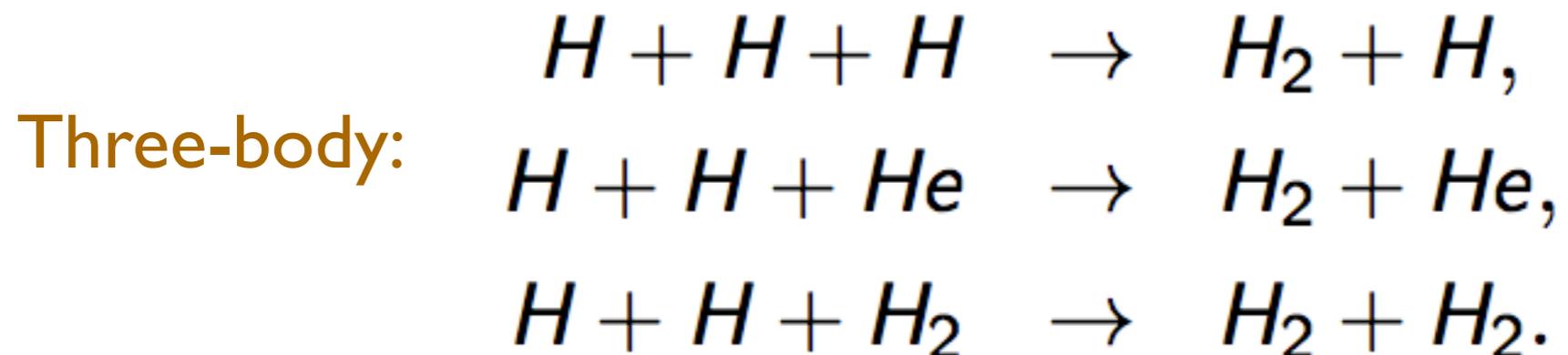
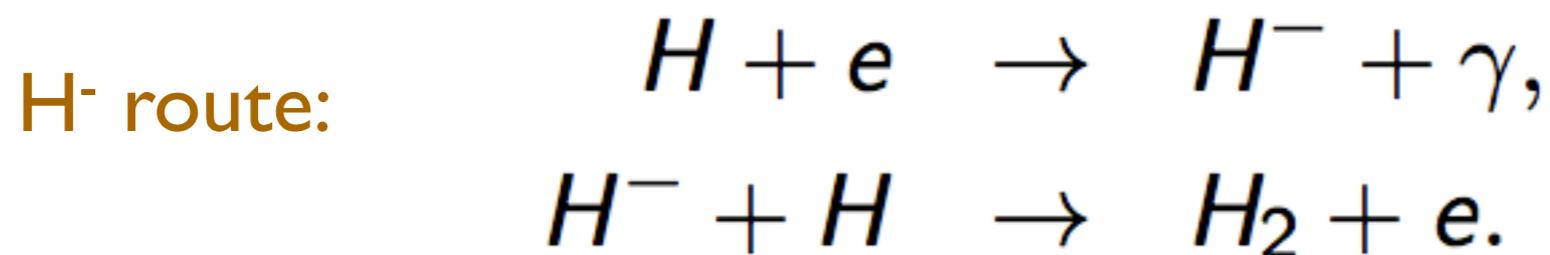
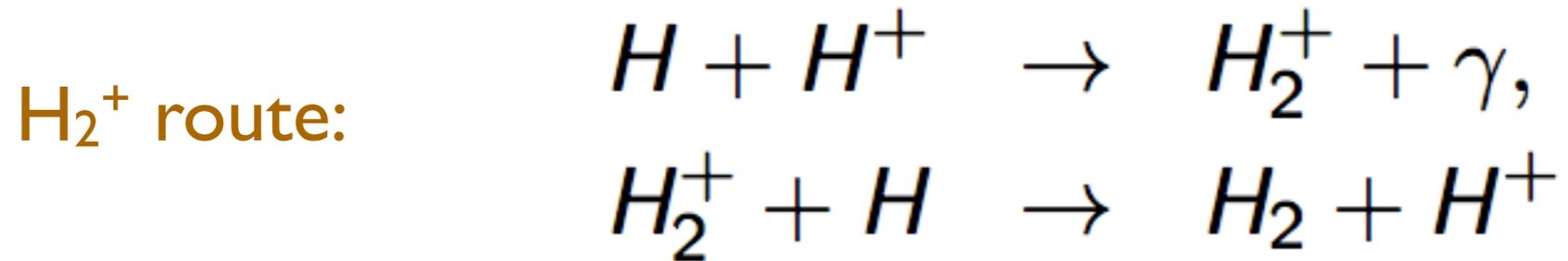
The ionization degree can only decrease
until $t_{rec} \sim t_{dyn}$.

Result: $x_e \sim \rho^{-1/2}$

x_e will not reach its equilibrium value!

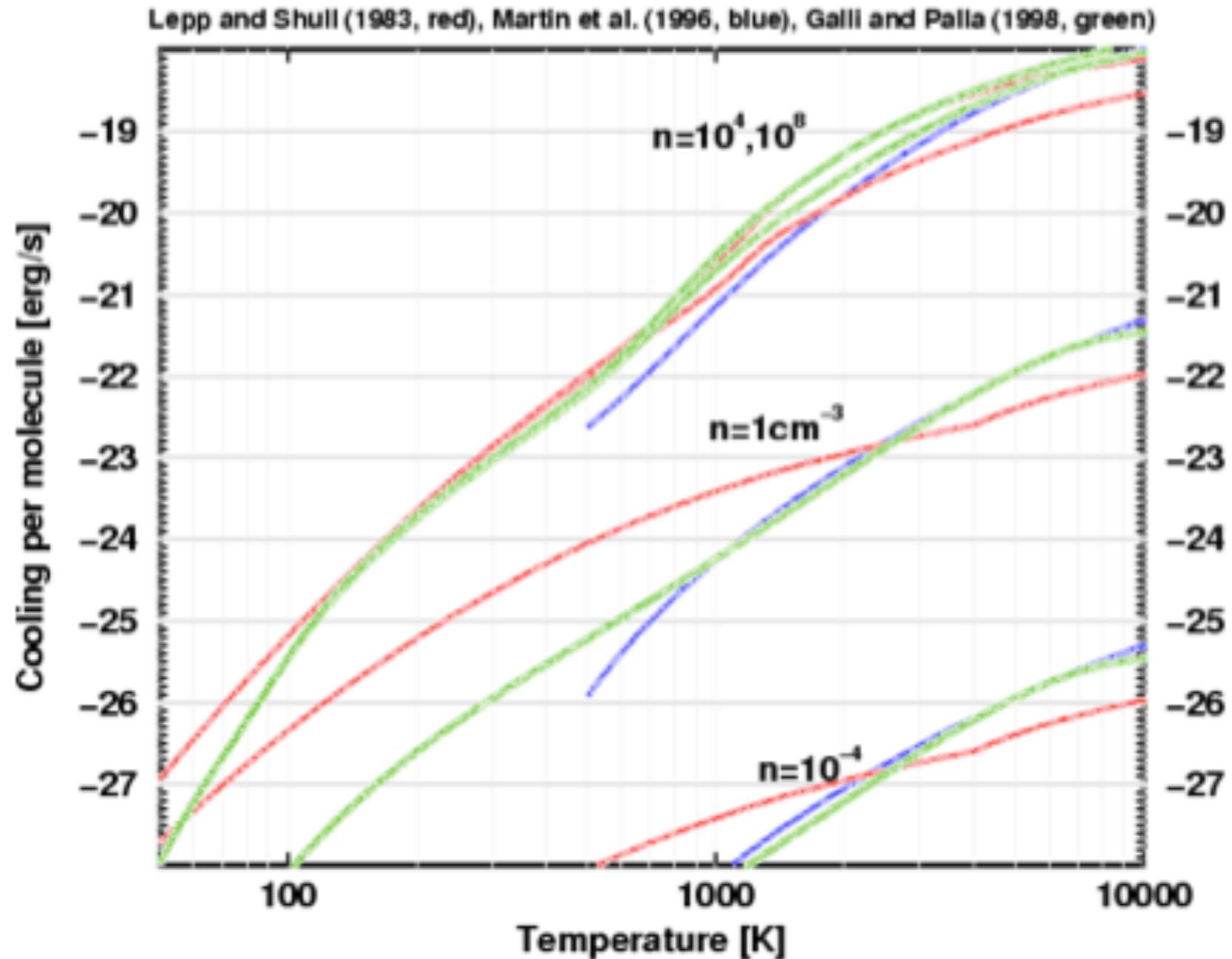
Formation of molecular hydrogen

A non-zero ionization degree triggers H₂ formation:



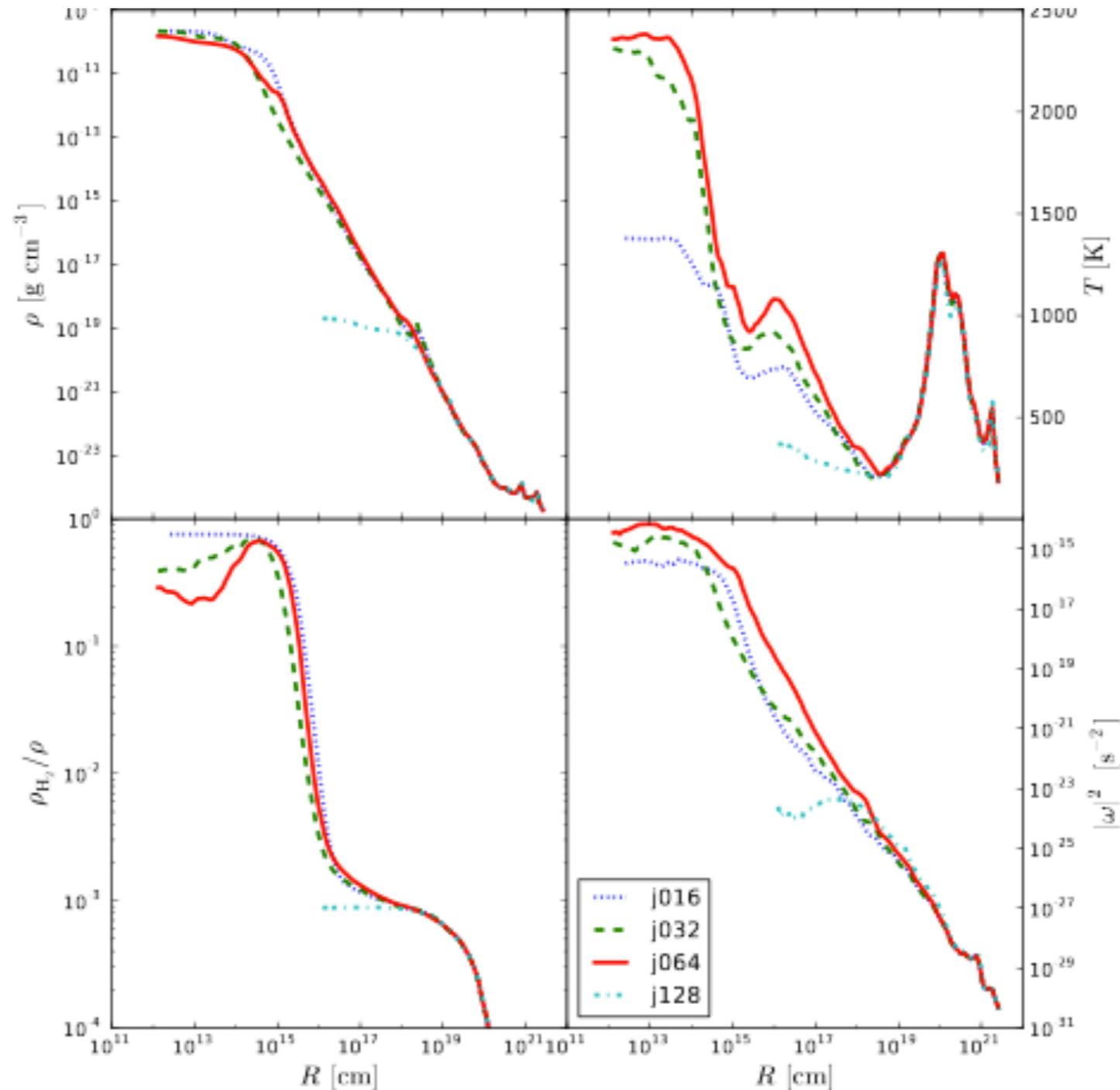
see talk D. Galli for detailed discussion

Cooling by molecular hydrogen



H_2 provides the path to cool below 10^4 K!

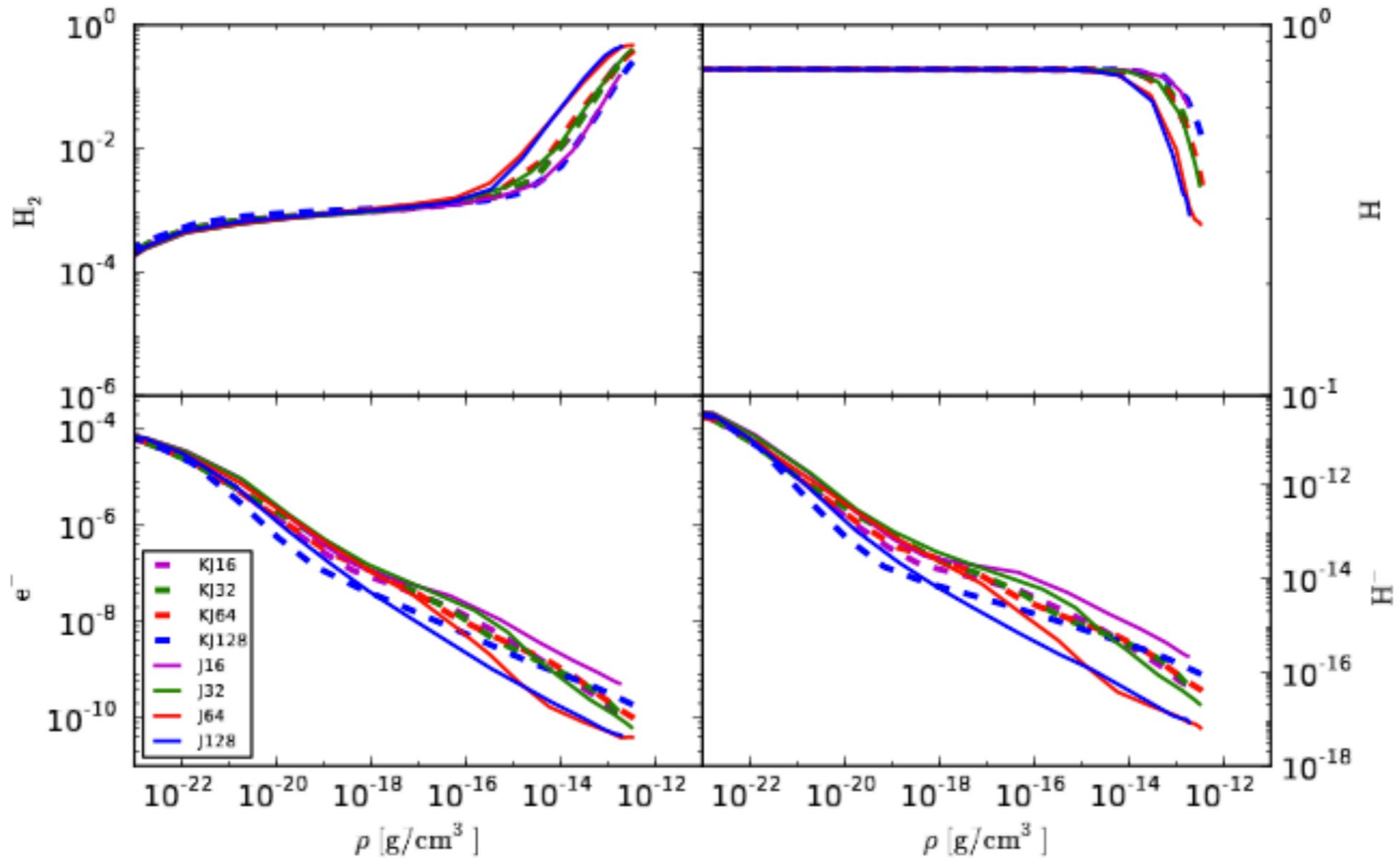
Primordial chemistry in high-resolution simulations



chemistry:
9 species,
20 reactions

Primordial chemistry solved with first-order solver
for different resolutions per Jeans length
(Turk et al. 2012)

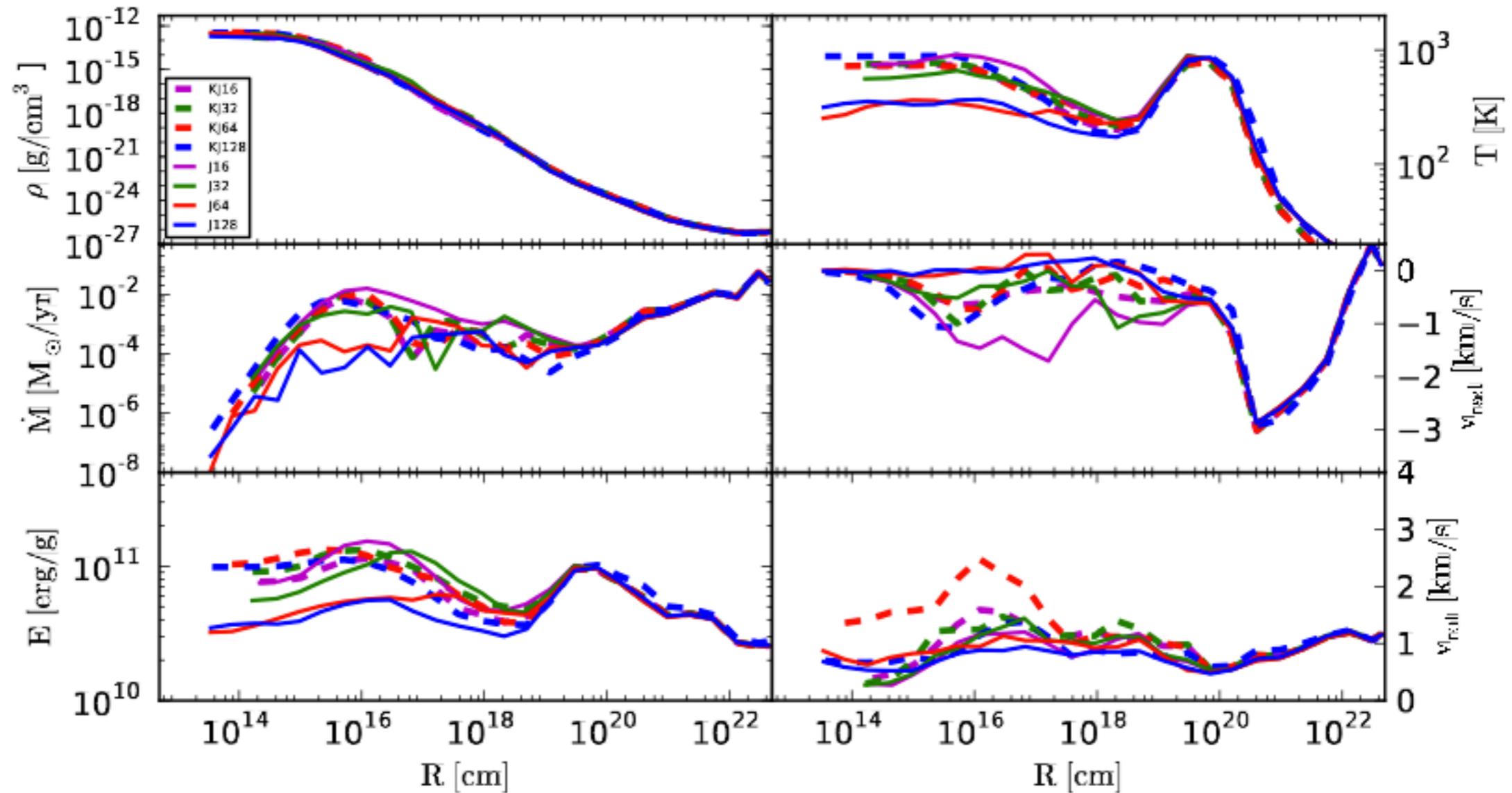
Importants of high-order methods



KROME results (dashed line) converged,
large scatter in first-order BDF

Bovino et al. (2013)

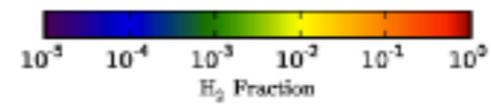
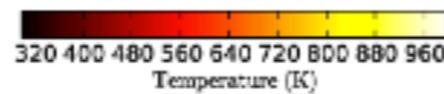
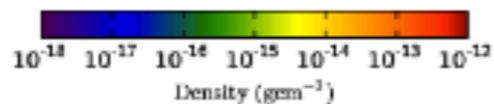
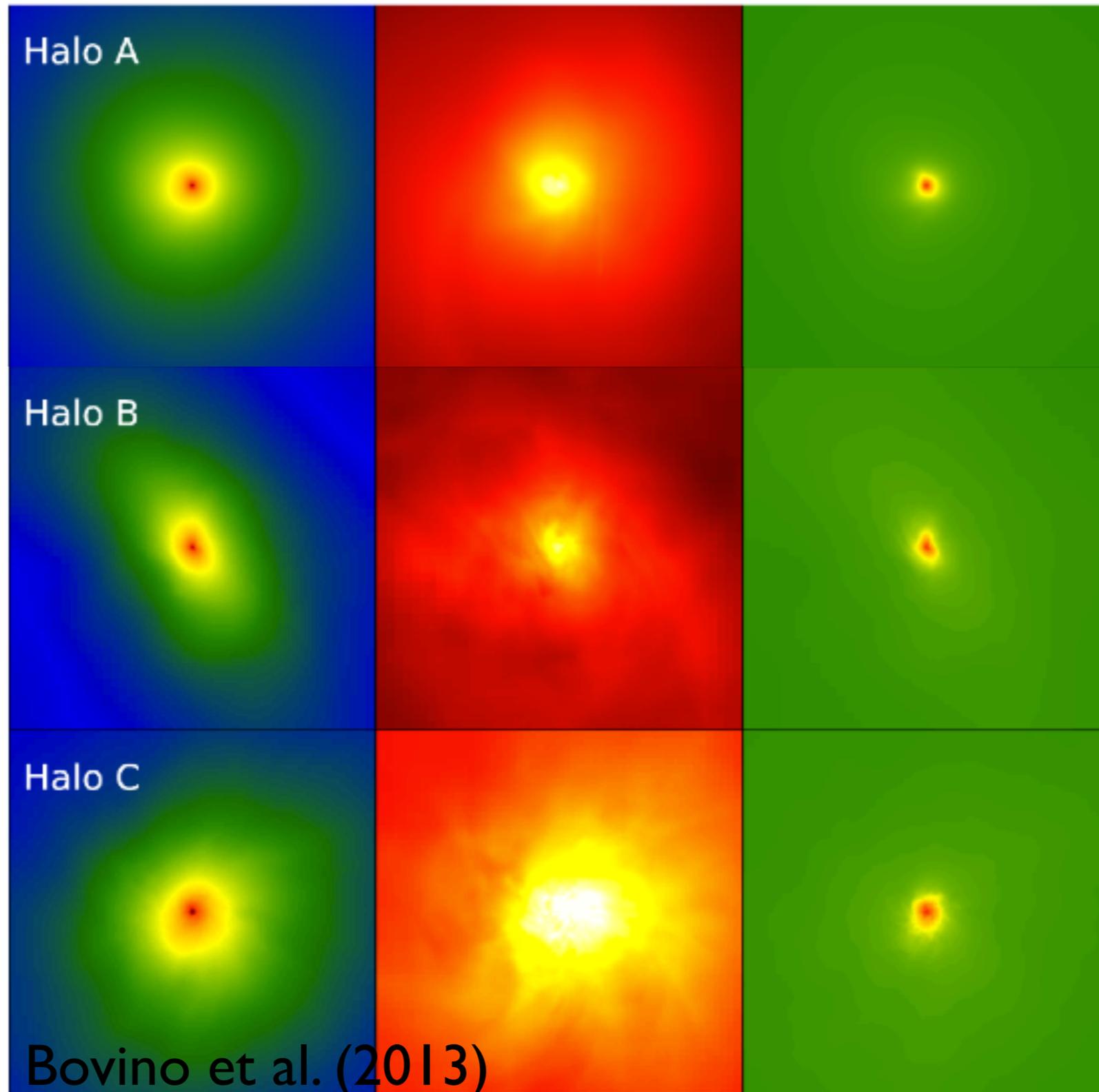
Importants of high-order methods



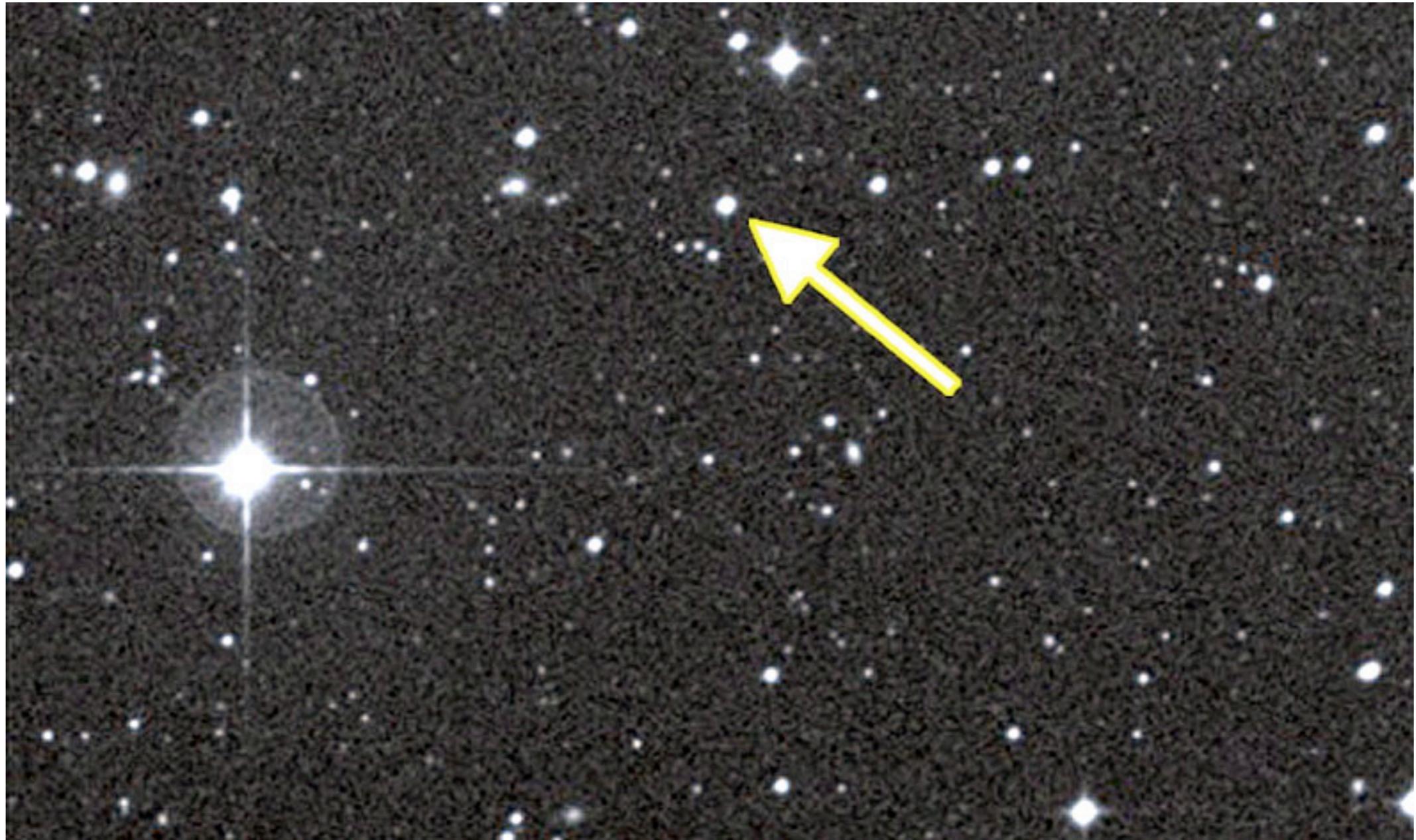
Convergence of chemistry leads to convergence of hydrodynamics (KROME: dashed line)

Bovino et al. (2013)

Density, temperature and chemical structure

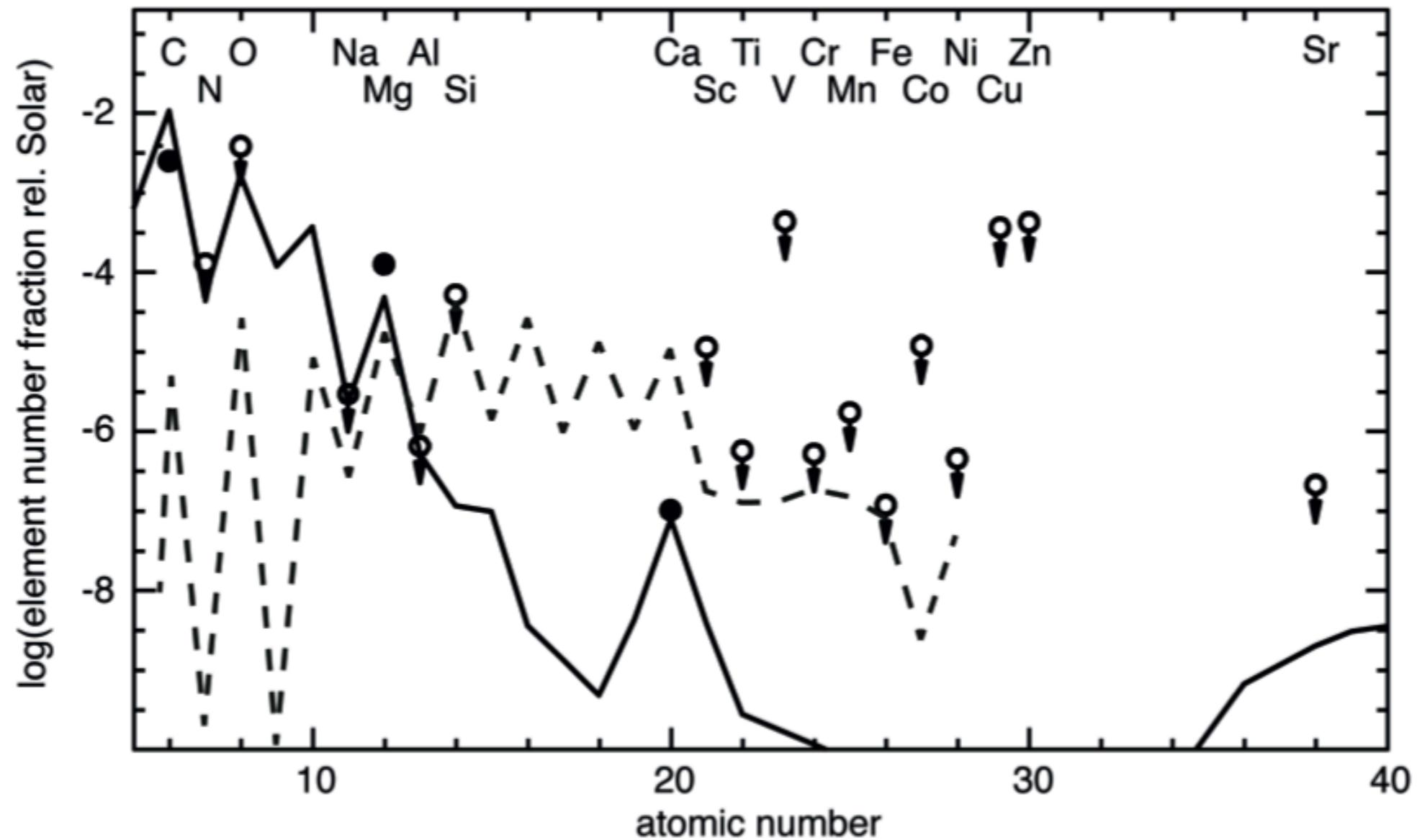


The extremely metal-poor star SMSS J031300.36-670839.3



The oldest-known star in the Milky Way with an age of 13.6 billion years
(formation: 100 million years after the Big Bang).

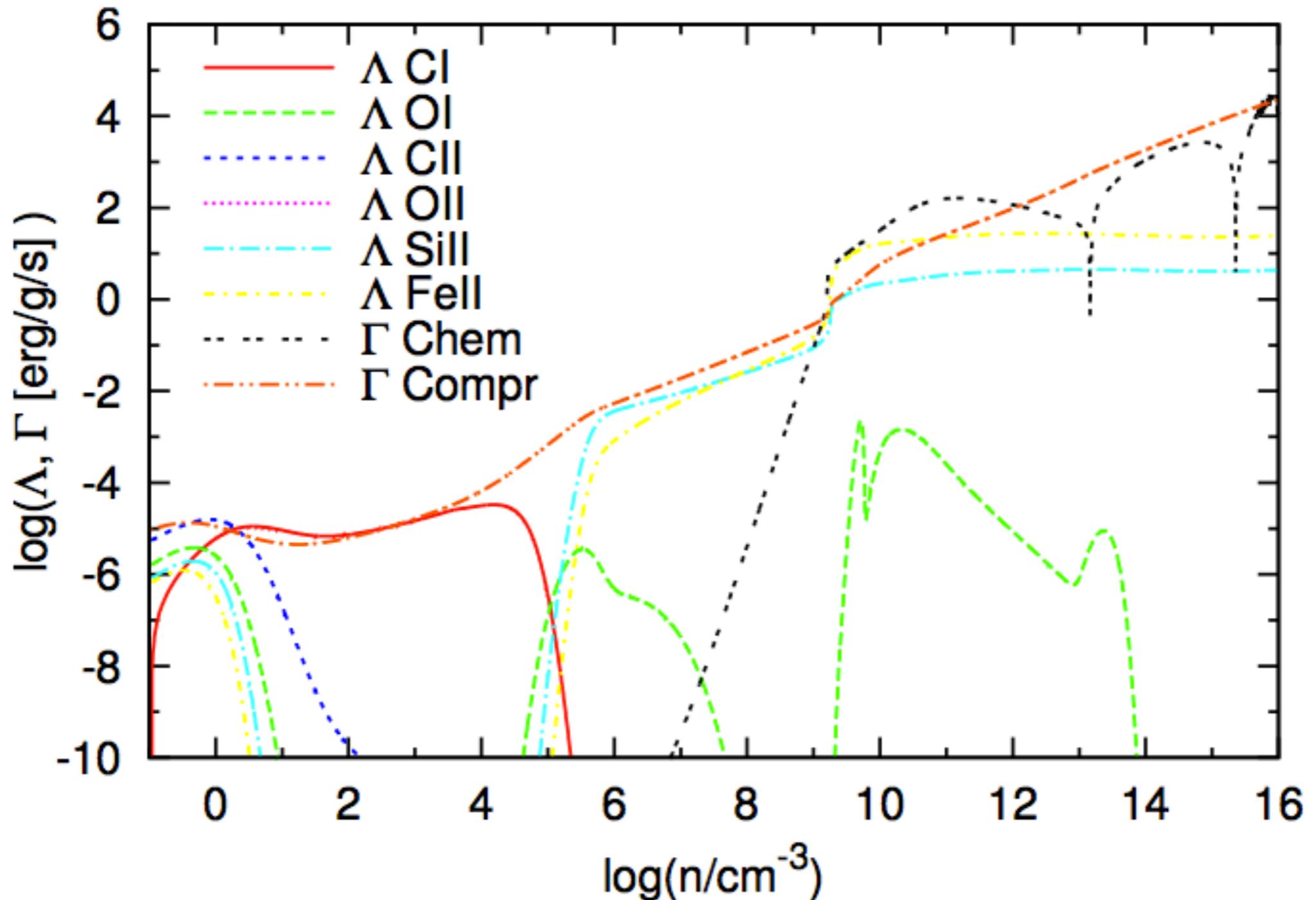
Metal abundances in SMSS J031300.36-670839.3



The composition of the star is consistent with one single supernova for metal enrichment and tells us the chemical initial conditions.

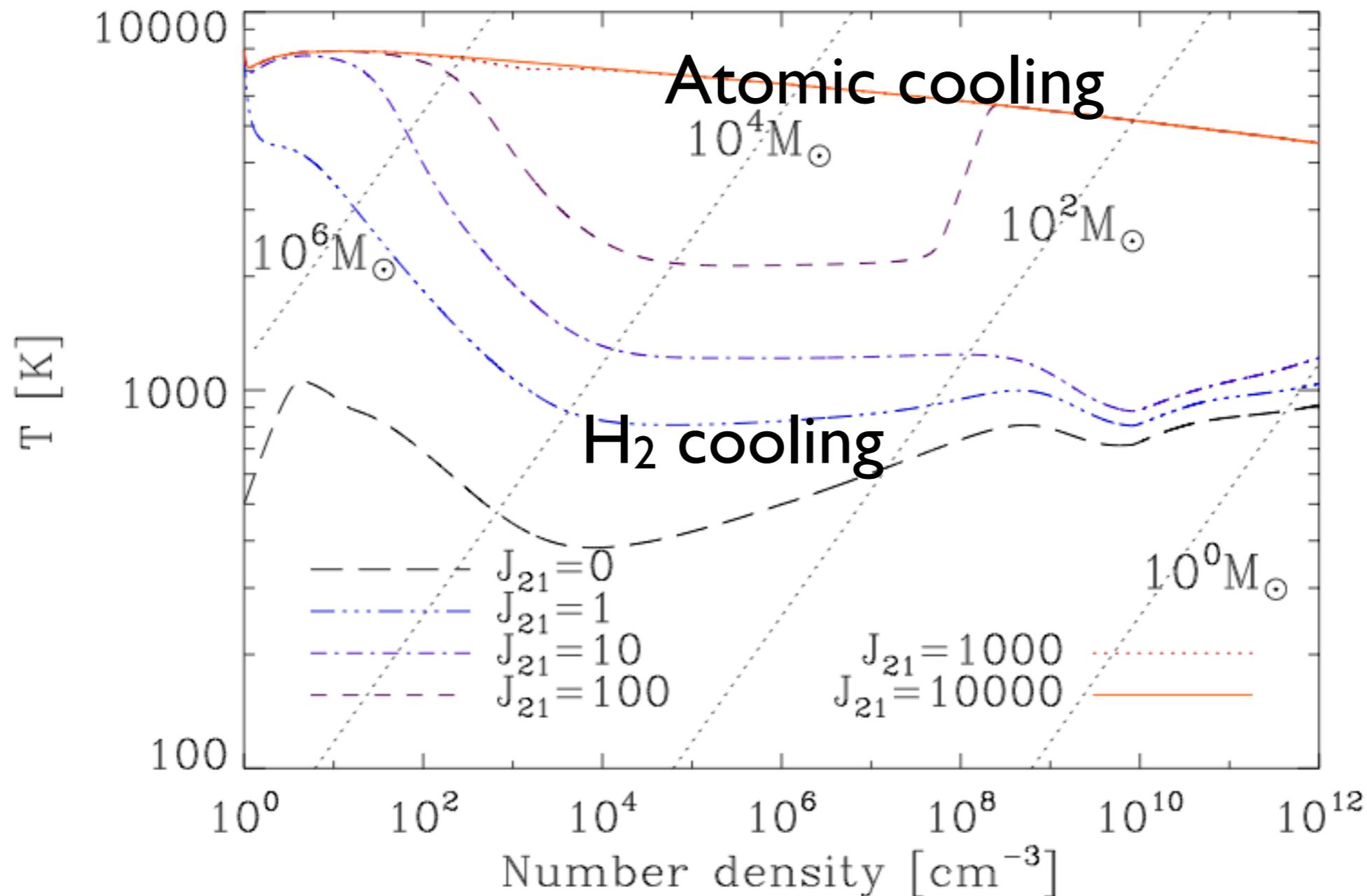
Keller et al. (2014)

Metal cooling in KROME



The public version already includes cooling via metals (Grassi et al. 2014).

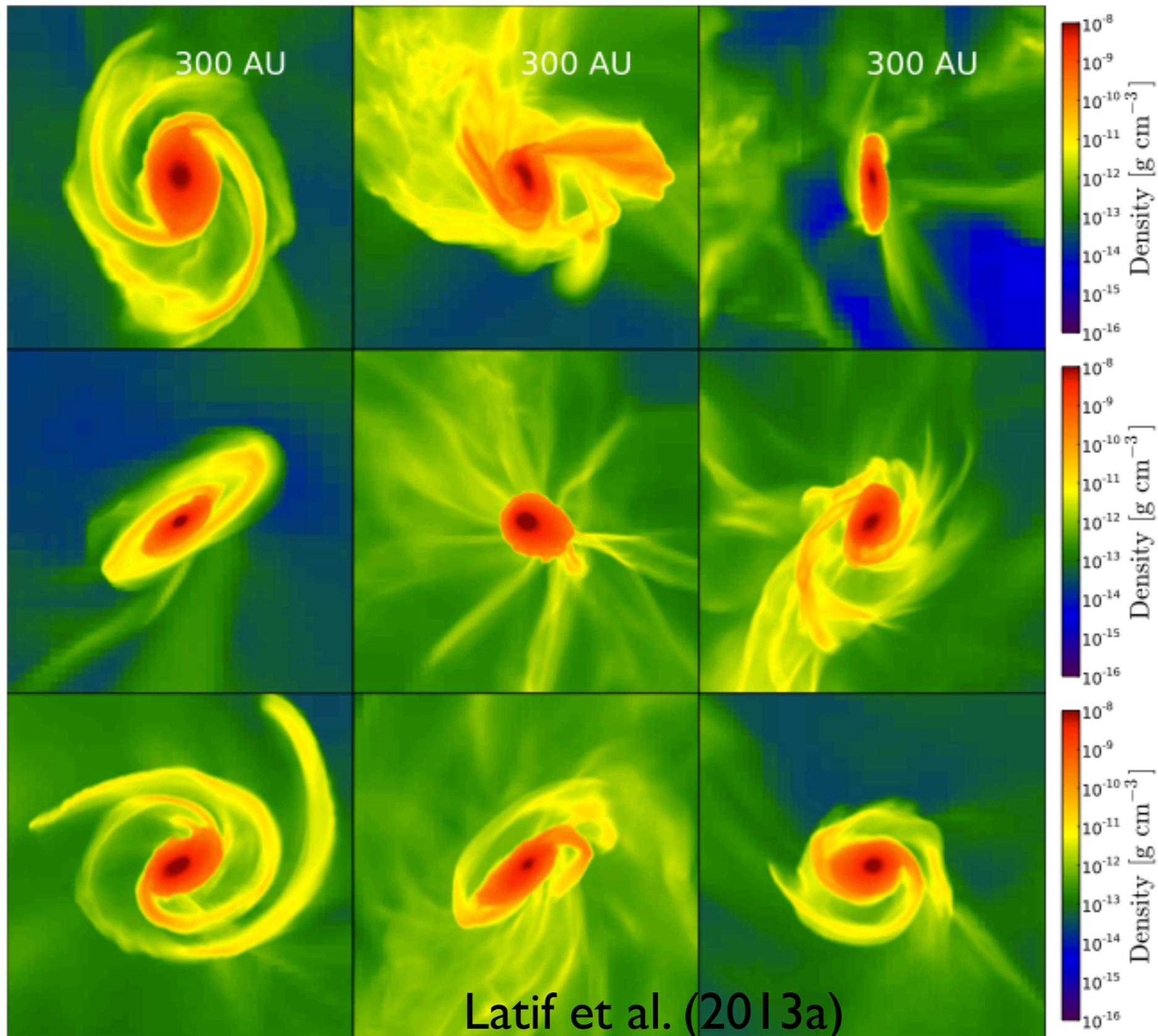
Thermodynamics in primordial gas



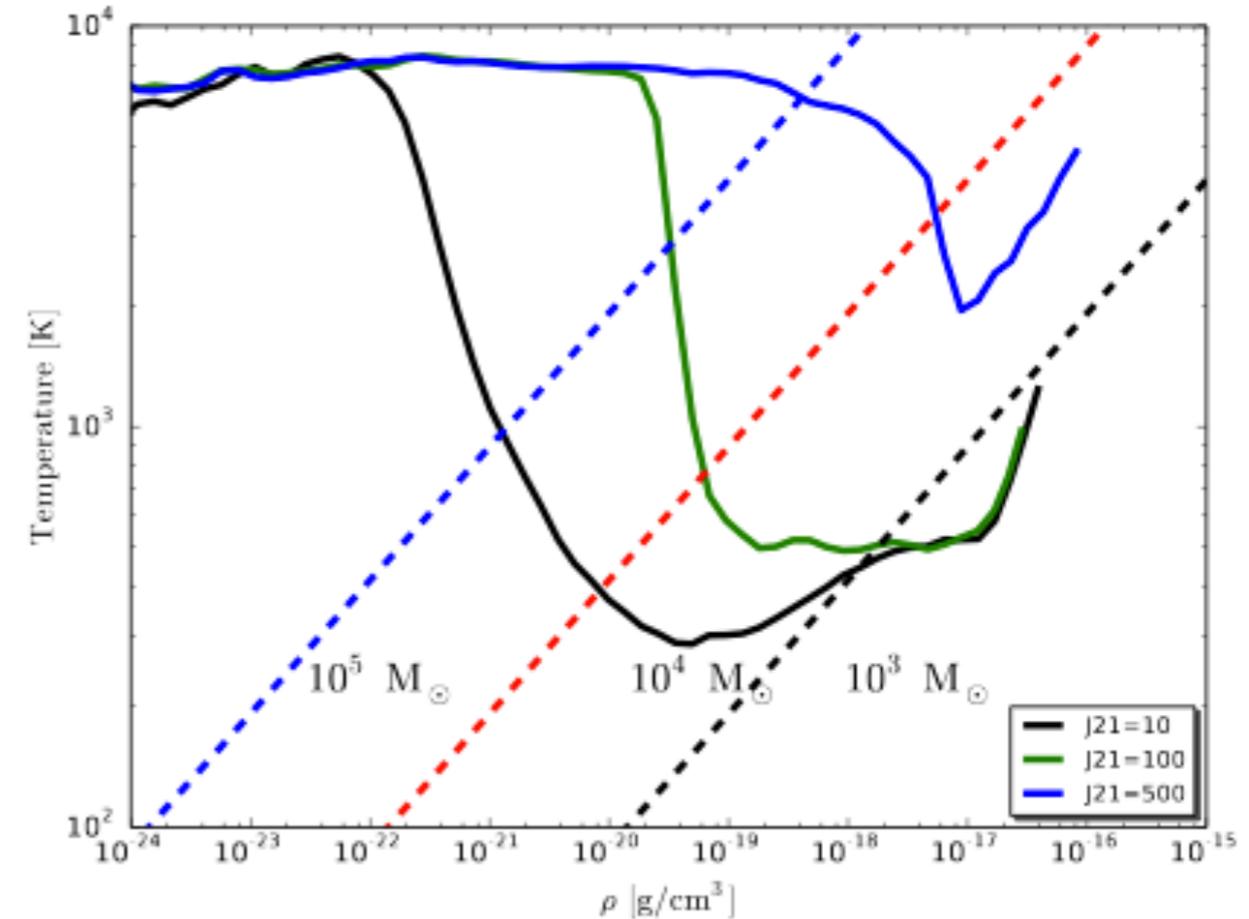
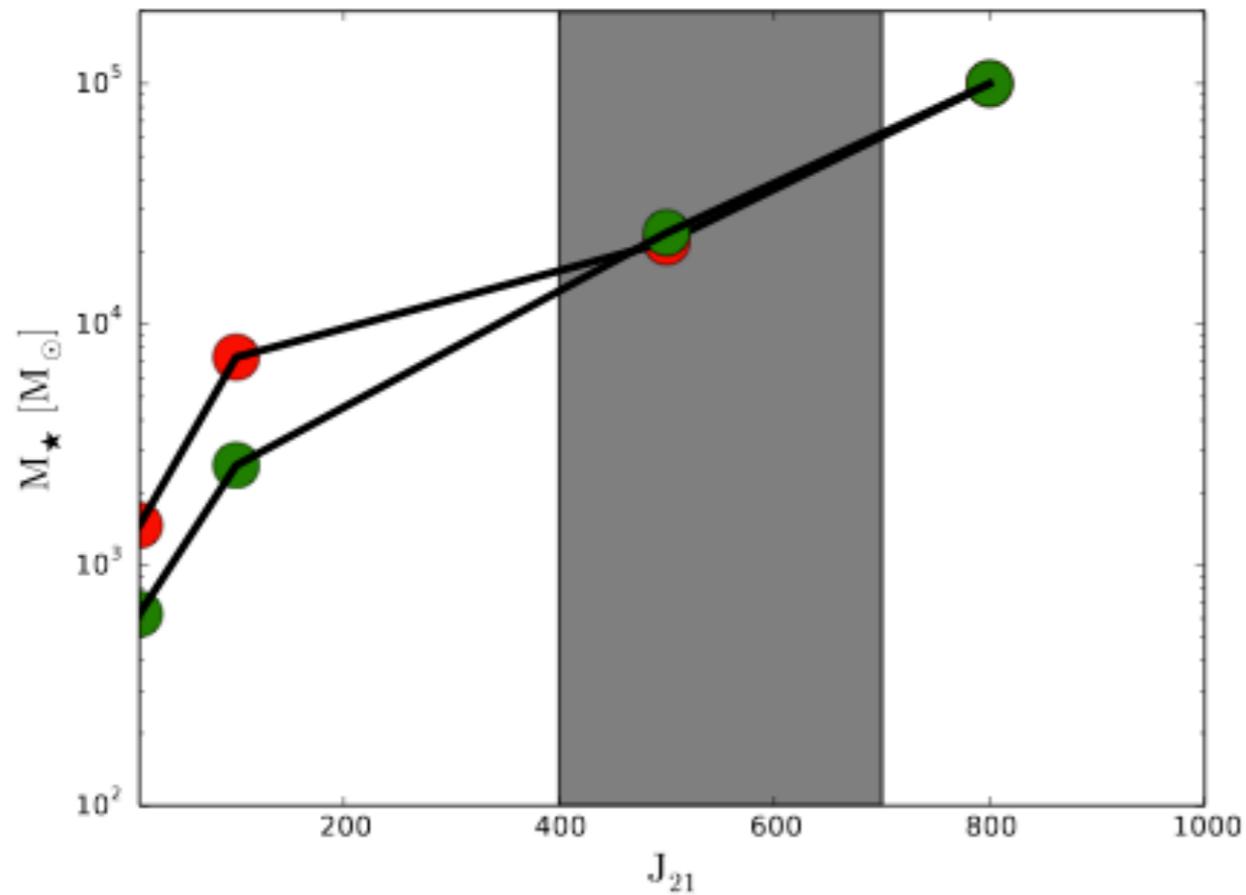
UV radiation: $J(\nu) = J_{21} \times 10^{-21} \frac{B_{\nu}(T_r)}{B_{\nu,H}(T_r)} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ sr}^{-1} \text{ Hz}^{-1}$

Schleicher, Spaans & Glover (2010)

Formation of supermassive black holes (I)



Formation of supermassive black holes (2)



UV radiation field:
$$J(\nu) = J_{21} \times 10^{-21} \frac{B_\nu(T_r)}{B_{\nu,H}(T_r)} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ sr}^{-1} \text{ Hz}^{-1}$$

Latif, Schleicher, Bovino, Grassi & Spaans (2014)

Summary

- Chemistry should be included in hydrodynamical simulations for the **dynamical modeling** and to foster the **comparison with observational data**.
- The advection is treated via **hydrodynamics**, the **chemistry** via KROME:
- A **high-order treatment** is required for high-resolution simulations.
- **Current applications include:**
formation of primordial stars, low-metallicity stars, supermassive black holes, protoplanetary disks, galaxy mergers

Enjoy the school!