Computational Astrophysics

5b. Microphysics – Context

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- Basically it’s everything happening inside a cell, on scales below the resolution

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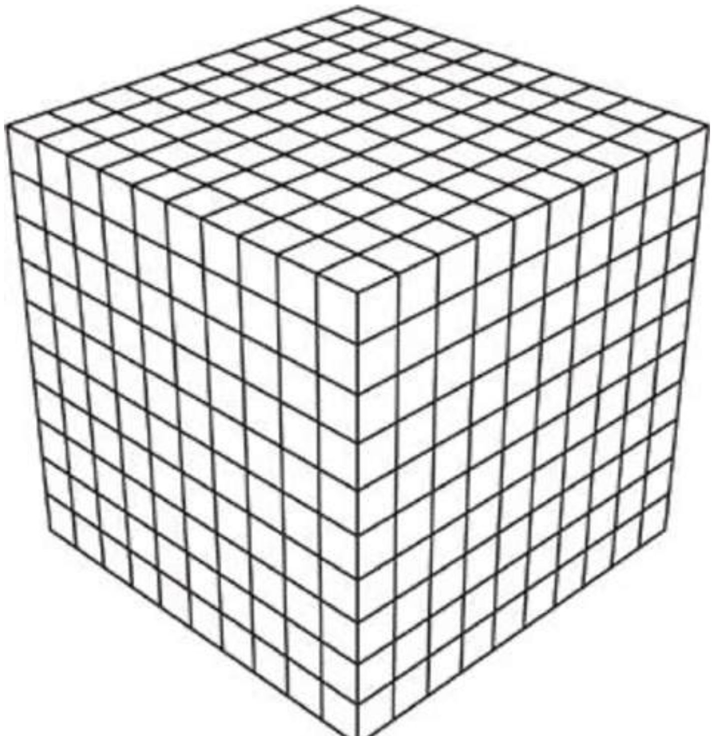

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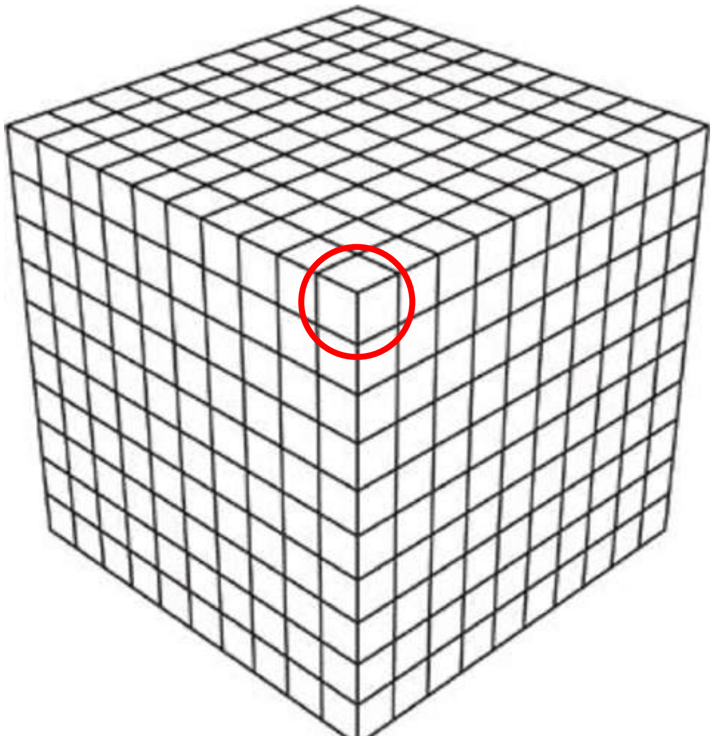

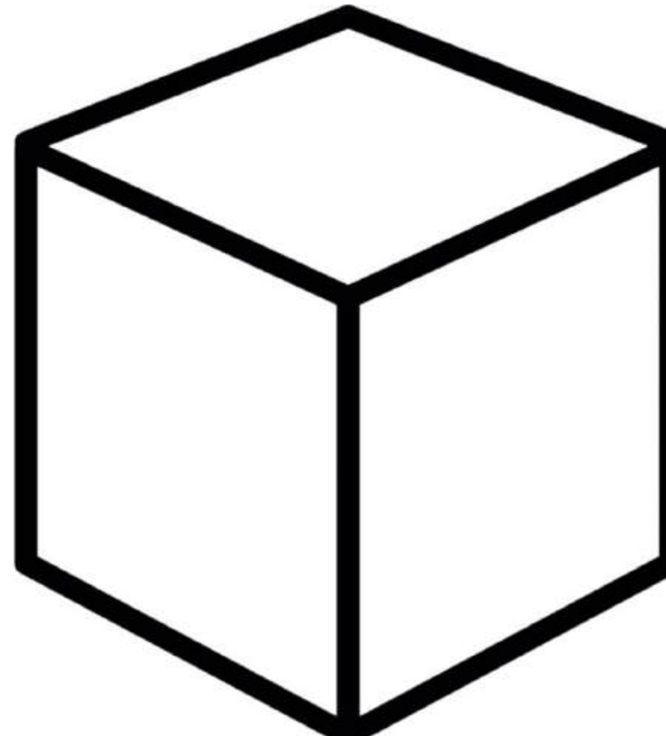

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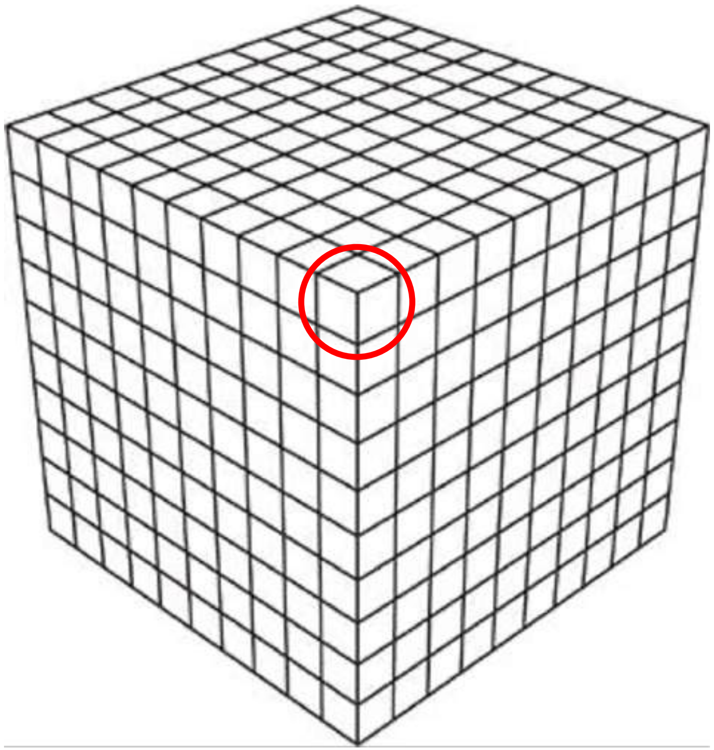

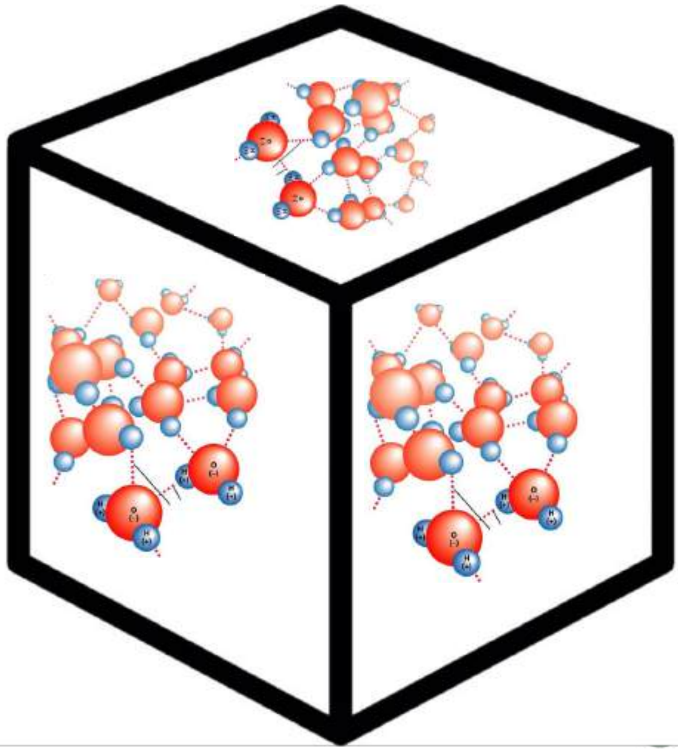

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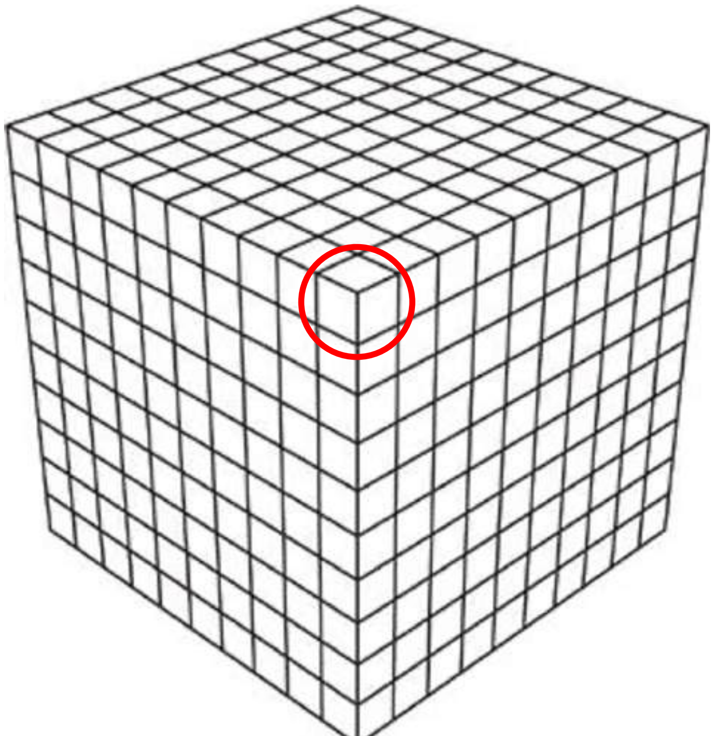

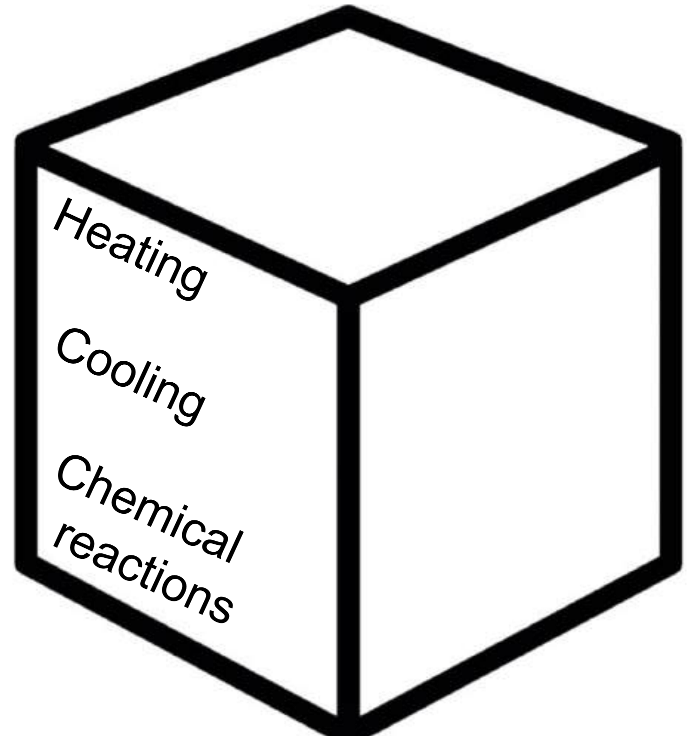

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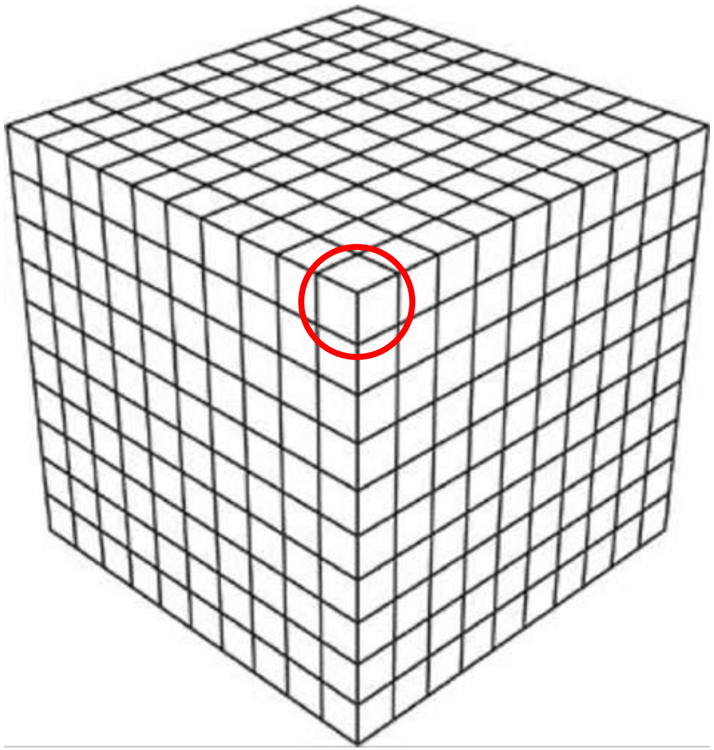

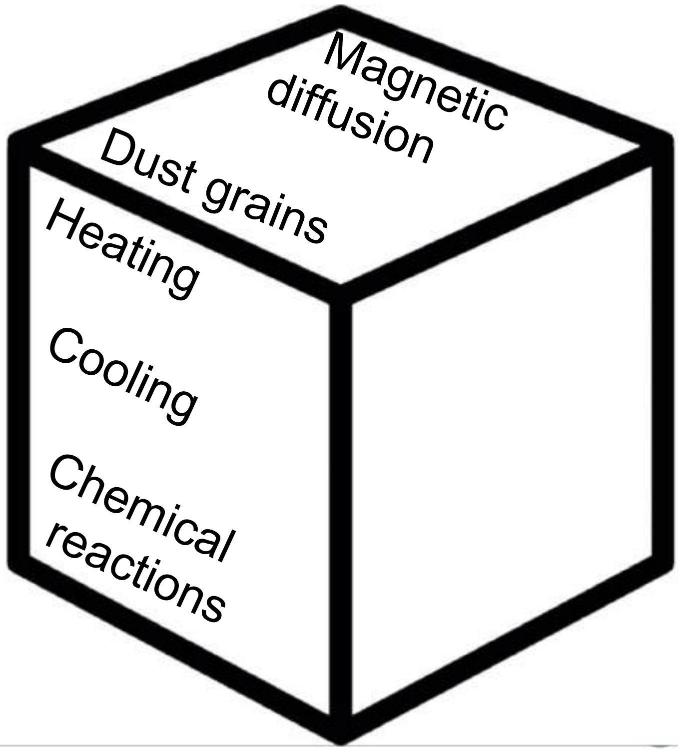

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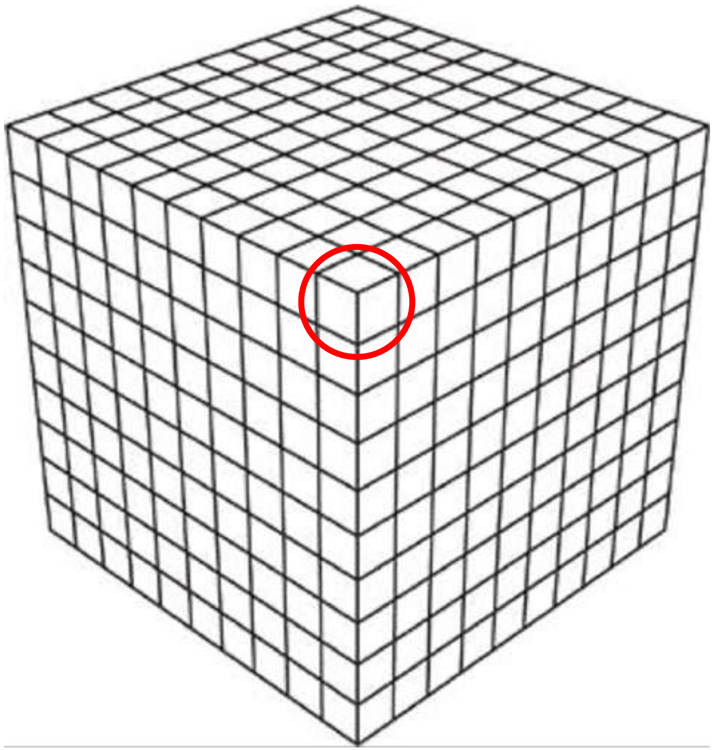

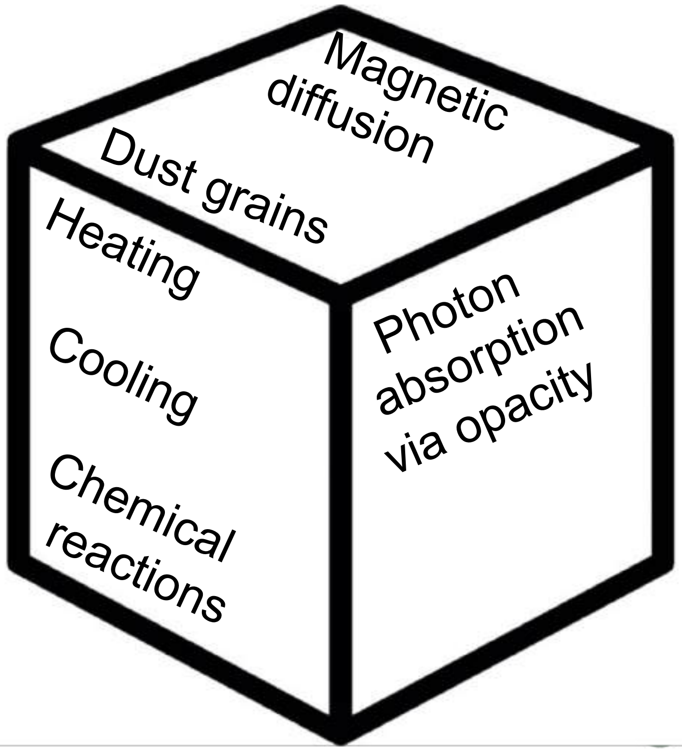

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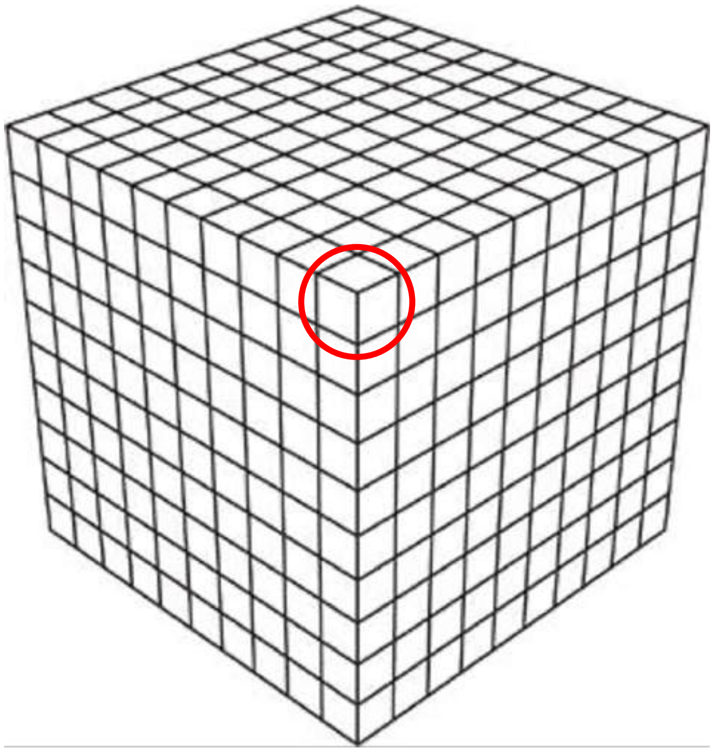
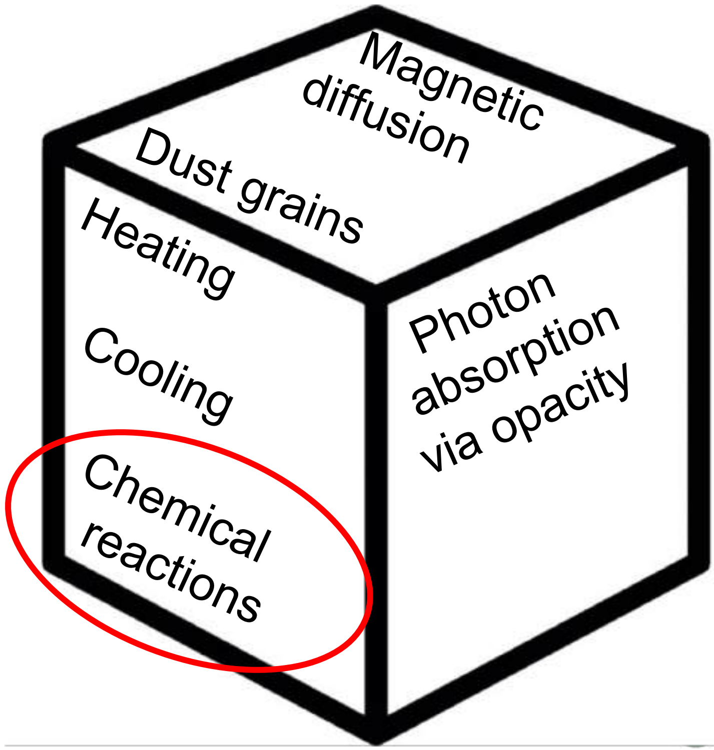
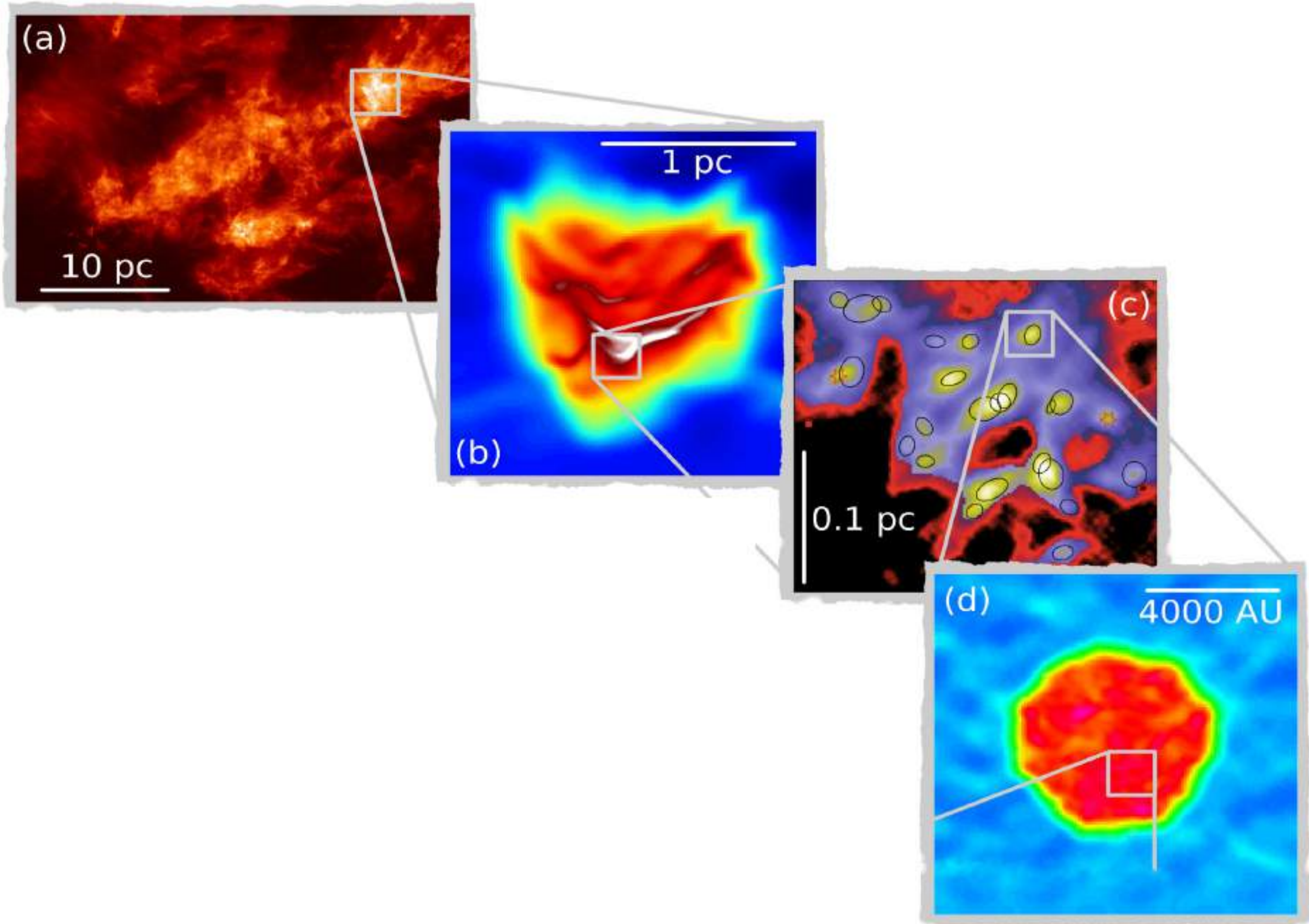




Why do we need Astrochemistry ?

- As an **observational diagnostic**:
  - H_2, CO, H_2O, O_2, CH are common molecules found in the ISM
  - Molecular ***rotational and vibrational bands*** can be observed at infrared to mm wavelengths
  - The molecular bands trace indirectly the density, temperature, etc. ***probing the physical state*** of the gas in the clouds
- For **modelling thermal processes**:
  - The ***equation of state*** depends on the chemical abundances
  - ***Heating and cooling*** is directly related to the chemistry
  - ***Ionization and conductivity*** depend on having a reservoir of free electrons and ions

Thermal Structure in protostellar collapse



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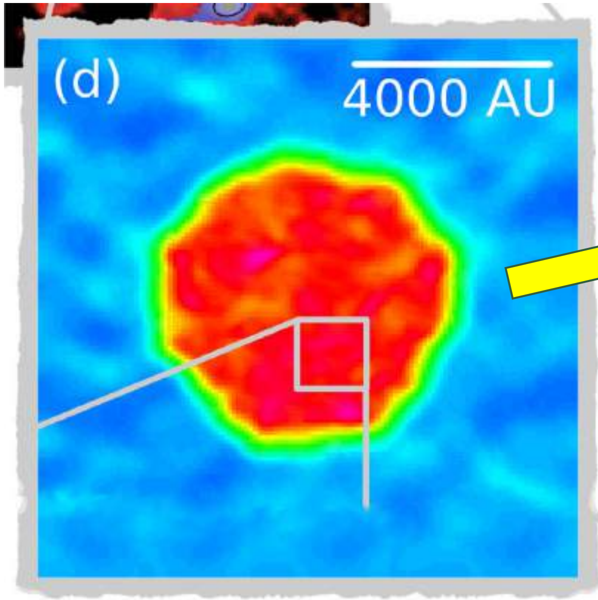

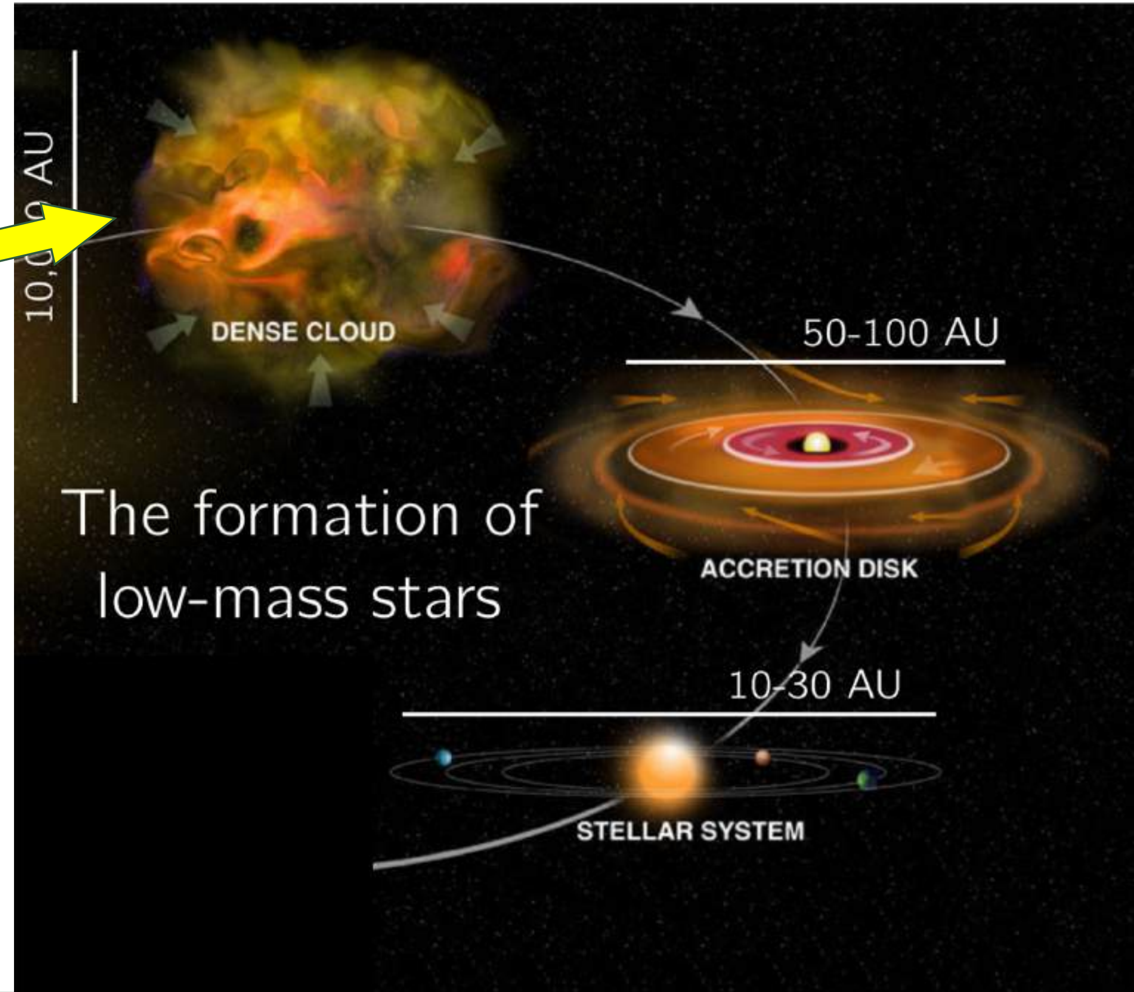

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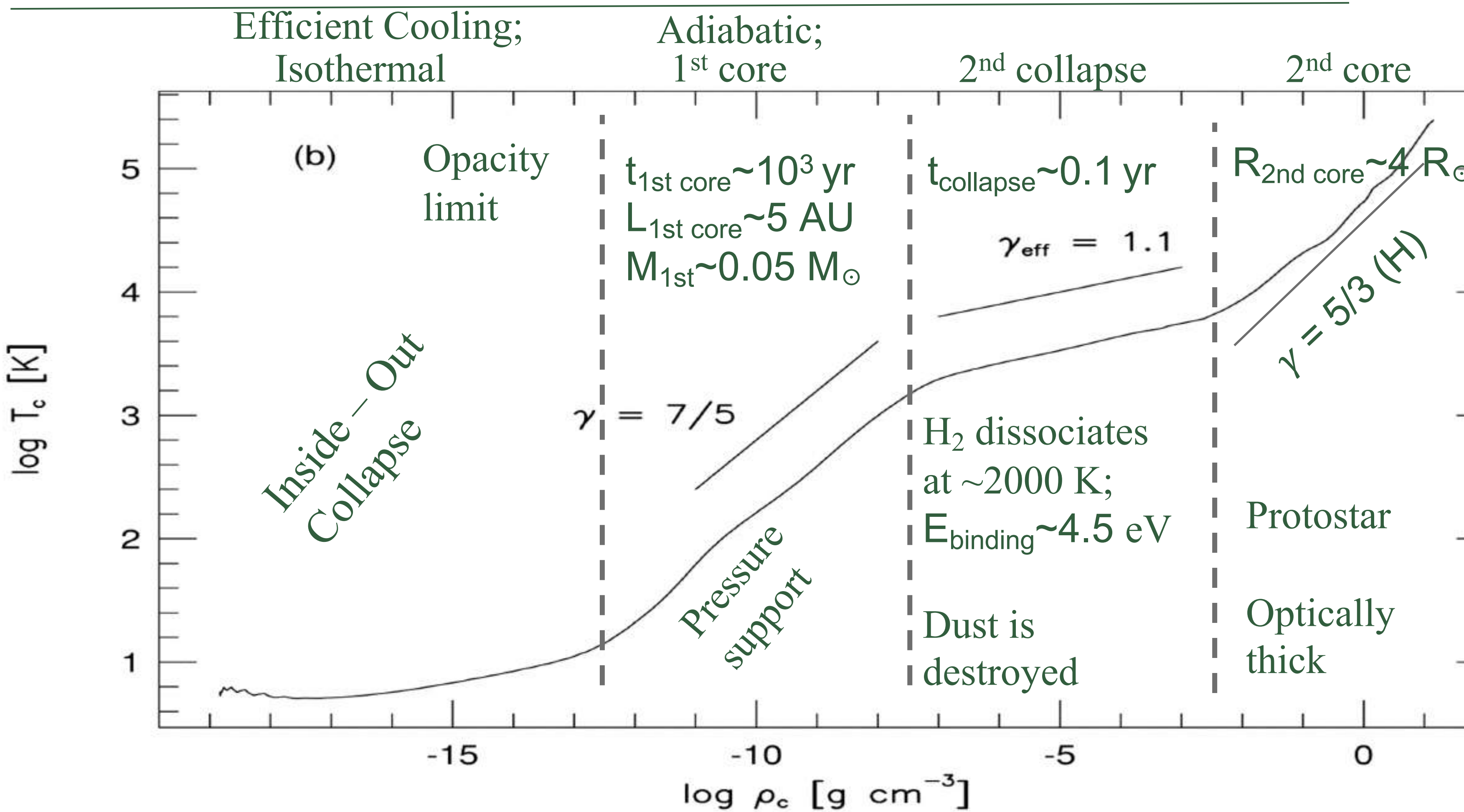
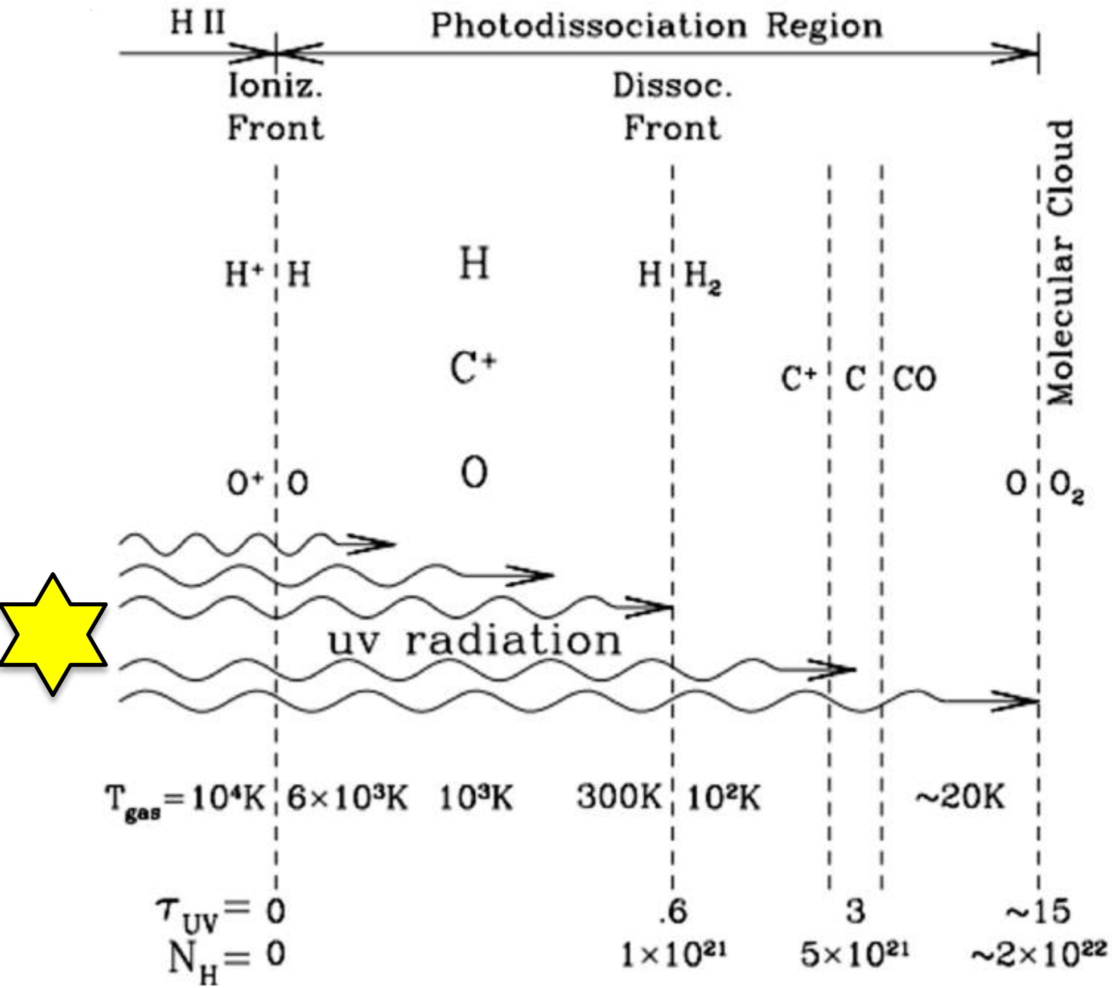
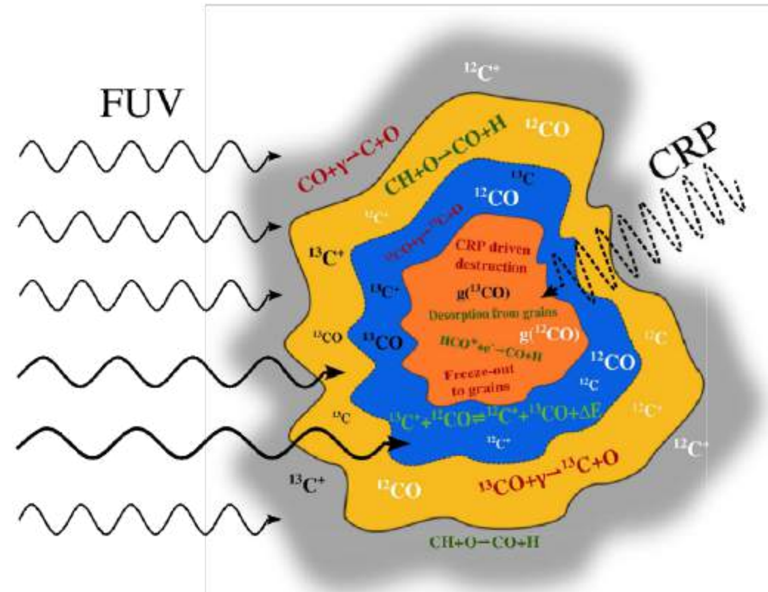


[Masunaga & Inutsuka 2000 – but already described in Larson '69!]

Thermal Structure near massive stars – PDRs



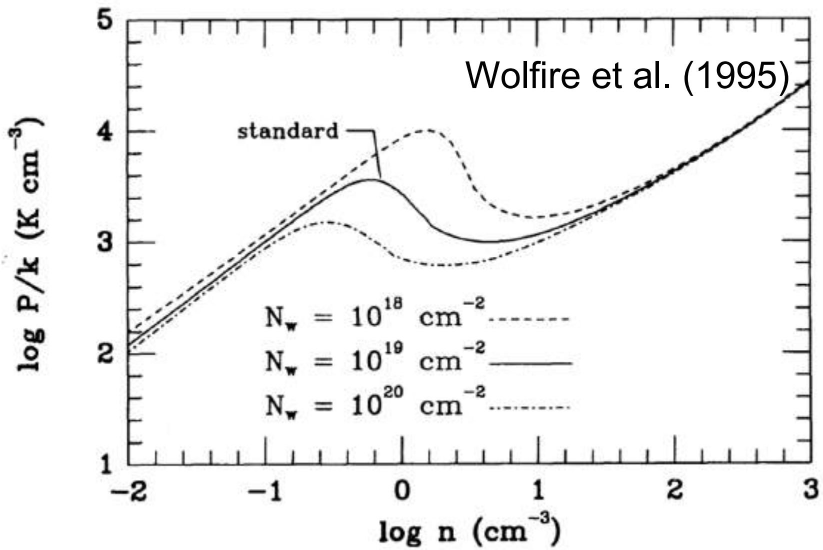
[Draine and Bertoldi 99]



[Szűcs et al. 14]

Thermal balance in the ISM

- The state of matter in the ISM depends on the ***balance between heating and cooling***.
- In principle, given a density, one can calculate the temperatures where these processes balance, resulting in a ***temperature-density diagram***.
- Although the ISM contains both 10^6 K gas (low density) and H_2 at ~10 K (high density), the ***different phases are roughly in pressure balance.***



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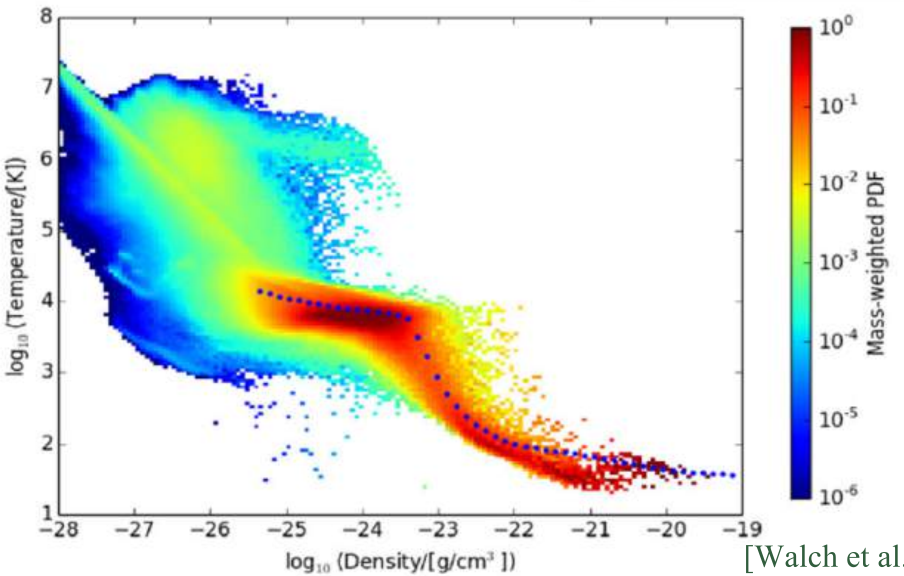

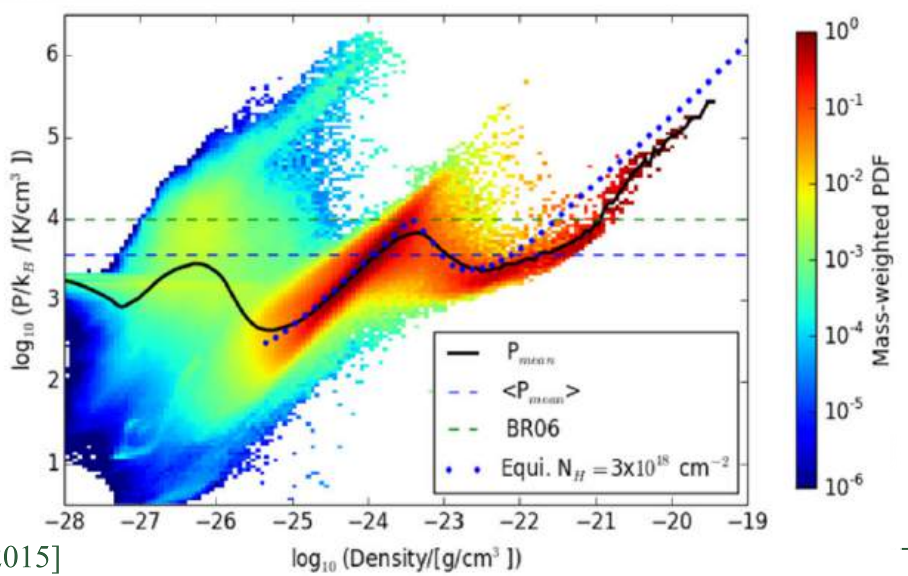

[Walch et al. 2015]

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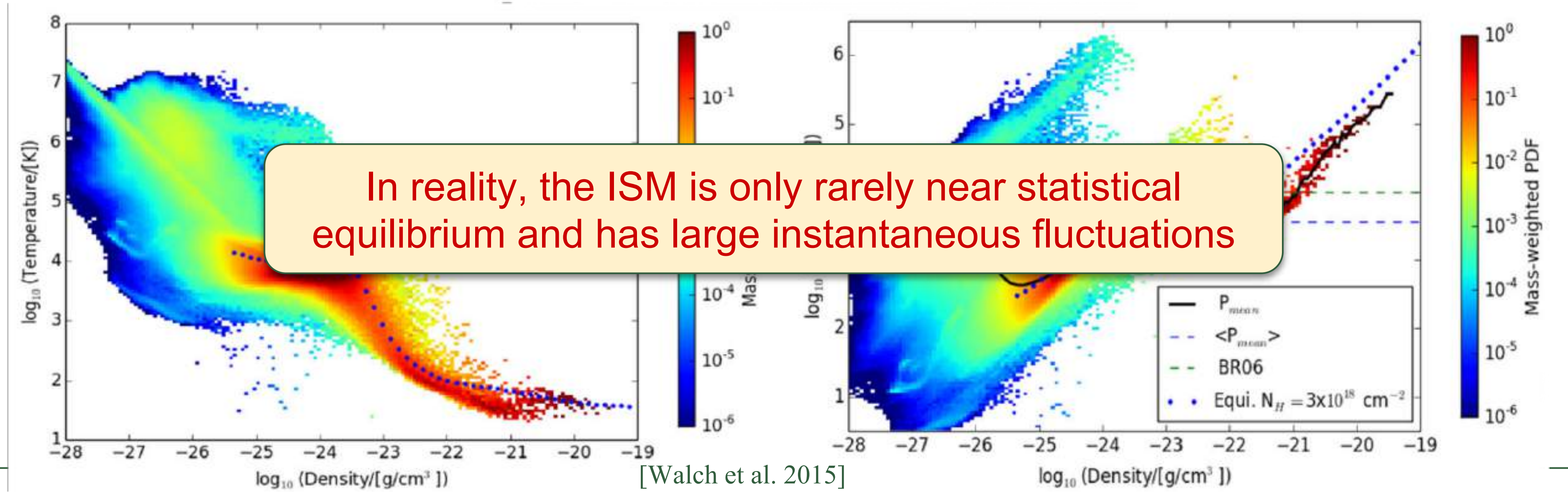


In reality, the ISM is only rarely near statistical equilibrium and has large instantaneous fluctuations

[Walch et al. 2015]

Thermal Evolution – Heating processes in MCs

- CMB radiation at 2.73(1+z) K – important in early universe

$$\frac{\partial(\rho e_{\text{int}})}{\partial t} + \nabla(\rho e_{\text{int}}\mathbf{u}) + P\nabla\cdot\mathbf{u} = Q_{stress} + Q_B - \nabla\cdot\mathbf{q}_B + Q_{heating} - \Lambda_{cooling}$$

- Cosmic-ray absorption

  $Q_{CR} \sim 10^{-27}\ n_H$ erg s^{-1} cm^{-3}

- Compressional heating
- Photo-Ionization in UV and X-rays
  - from massive stars
  - close to protostars
- Photo-electric heating through dust
  - Photon frees electron; ionize molecules

Thermal Evolution – Cooling processes

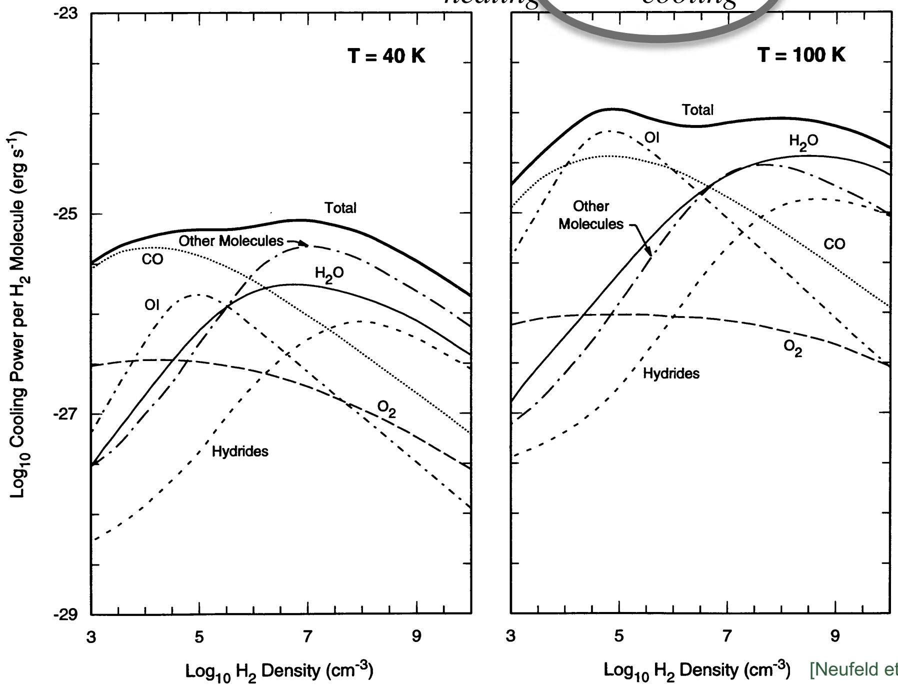
$$\frac{\partial(\rho e_{\rm int})}{\partial t} + \nabla(\rho e_{\rm int}\mathbf{u}) + P\nabla\cdot\mathbf{u} =$$
$$Q_{stress} + Q_B - \nabla\cdot\mathbf{q}_B$$
$$+ Q_{heating} - \Lambda_{cooling}$$

- Collisional excitation with electrons followed by radiative decay dominant

  $\Lambda_{\rm cool} = n_{\rm ion}\, n_e\, \Delta E \sim n^2$

  - Has to be in forbidden lines, or else photons are reabsorbed
  - At higher temperatures (~100 K) atomic cooling dominates (CII,OI)
  - At low temperature / high density molecular rotational and vibrational bands are important (CO, H_20 etc). Collision with H_2.
  - Complicated to calculate

- Cooling by dust vibration (IR)
- Chemical cooling – e.g. H_2 dissociation, H ionization; works like a phase transition.



[Neufeld et al 95]

Numerical Implementation - Heating

- *Cosmic ray heating* is constant, and proportional to density (except maybe everywhere: suppressed in protostars, enhanced near production sources, inhomogeneous on galactic scales).
  - $Q_{CR} \sim 10^{-27}\ n_H$ erg s^{-1} cm^{-3}
- *Interactions with photons* – proportional to flux and density
  - Photo-electric heating through dust grains
  - Photo-electric heating by UV $\quad Q_{HEAT} = 4\pi \int d\nu\, \rho\, \kappa_\nu\, J_\nu = \Gamma_{HEAT} n_H$
  - Photo-electric heating by X-rays

→ In general, depends on calculating the flux; *next year!*

- Alternatively, assume an external flux, and an extinction relation:

$$F \sim F_{\mathrm{external}} \exp[-A_V]$$

- *Compressional heating:* Integrated in to the fluid equations
- *Chemical heating:* Part of a proper astro-chemistry treatment

Numerical Implementation - Cooling

- The standard approach for cooling in the interstellar medium is to use a table lookup, and assume that the cooling rates (per H atom)^2 is a function of temperature alone
- A more sophisticated approach is to have one table per species

HEATING AND IONIZATION OF HI REGIONS

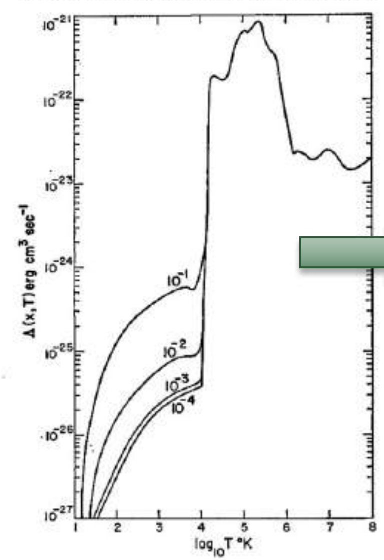
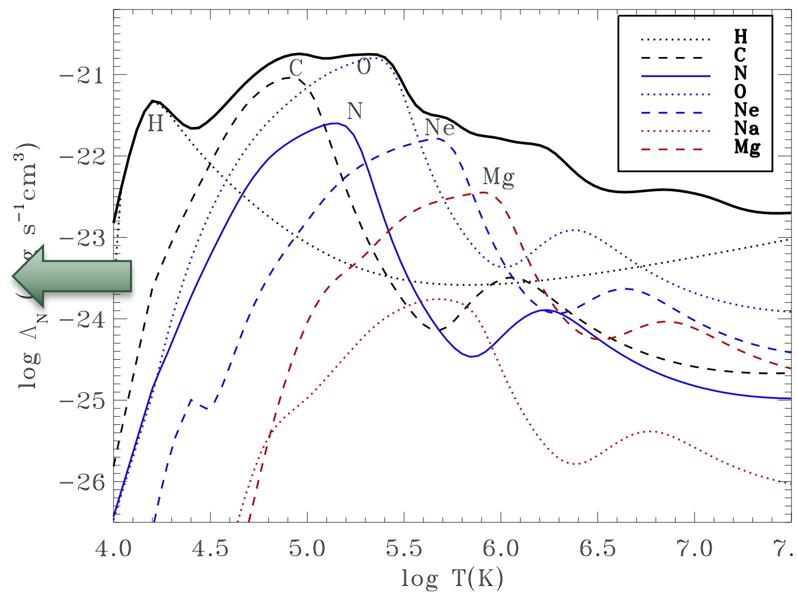


FIGURE 2. The interstellar cooling function $\Lambda(x, T)$ for various values of the fractional ionization x. The labels refer to the values of x.

[Dalgarno & McCray 1972]

log T (K)	log Λ_N (erg s^{-1} cm^3)	log Λ_{hd} (erg s^{-1} cm^3)	n_e/n_H
3.80	-25.7331	-30.6104	1.3264E-05
3.84	-25.0383	-29.4107	4.2428E-05
3.88	-24.4059	-28.4601	8.8276E-05
3.92	-23.8288	-27.5743	1.7967E-04
3.96	-23.3027	-26.3766	8.4362E-04
4.00	-22.8242	-25.2890	3.4295E-03
4.04	-22.3917	-24.2684	1.3283E-02
4.08	-22.0067	-23.3834	4.2008E-02
4.12	-21.6818	-22.5977	1.2138E-01
4.16	-21.4529	-21.9689	3.0481E-01
4.20	-21.3246	-21.5972	5.3386E-01
4.24	-21.3459	-21.4615	7.6622E-01
4.28	-21.4305	-21.4789	8.9459E-01
4.32	-21.5293	-21.5497	9.5414E-01
4.36	-21.6138	-21.6211	9.8342E-01
4.40	-21.6615	-21.6595	1.0046
4.44	-21.6551	-21.6426	1.0291
4.48	-21.5919	-21.5688	1.0547
4.52	-21.5092	-21.4771	1.0767
4.56	-21.4124	-21.3755	1.0888
4.60	-21.3085	-21.2693	1.0945
4.64	-21.2047	-21.1644	1.0972
4.68	-21.1067	-21.0658	1.0988
4.72	-21.0194	-20.9778	1.1004
4.76	-20.9413	-20.8986	1.1034
4.80	-20.8735	-20.8281	1.1102
4.84	-20.8205	-20.7700	1.1233
4.88	-20.7805	-20.7223	1.1433
4.92	-20.7547	-20.6888	1.1638
4.96	-20.7455	-20.6739	1.1791
5.00	-20.7565	-20.6815	1.1885
5.04	-20.7820	-20.7051	1.1937
5.08	-20.8008	-20.7229	1.1966
5.12	-20.7994	-20.7208	1.1983
5.16	-20.7847	-20.7058	1.1993
5.20	-20.7687	-20.6896	1.1999
5.24	-20.7590	-20.6797	1.2004
5.28	-20.7544	-20.6749	1.2008
5.32	-20.7505	-20.6709	1.2012
5.36	-20.7545	-20.6748	1.2015
5.40	-20.7888	-20.7089	1.2020
5.44	-20.8832	-20.8031	1.2025
5.48	-21.0450	-20.9647	1.2030
5.52	-21.2286	-21.1482	1.2035
5.56	-21.3737	-21.2932	1.2037
5.60	-21.4573	-21.3767	1.2039
5.64	-21.4935	-21.4129	1.2040
5.68	-21.5098	-21.4291	1.2041
5.72	-21.5345	-21.4538	1.2042
5.76	-21.5863	-21.5055	1.2044
5.80	-21.6548	-21.5740	1.2045
5.84	-21.7108	-21.6300	1.2046
5.88	-21.7424	-21.6615	1.2047
5.92	-21.7576	-21.6766	1.2049
5.96	-21.7696	-21.6886	1.2050

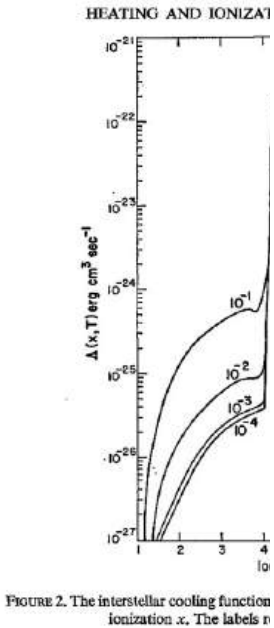


[Shure 2009]

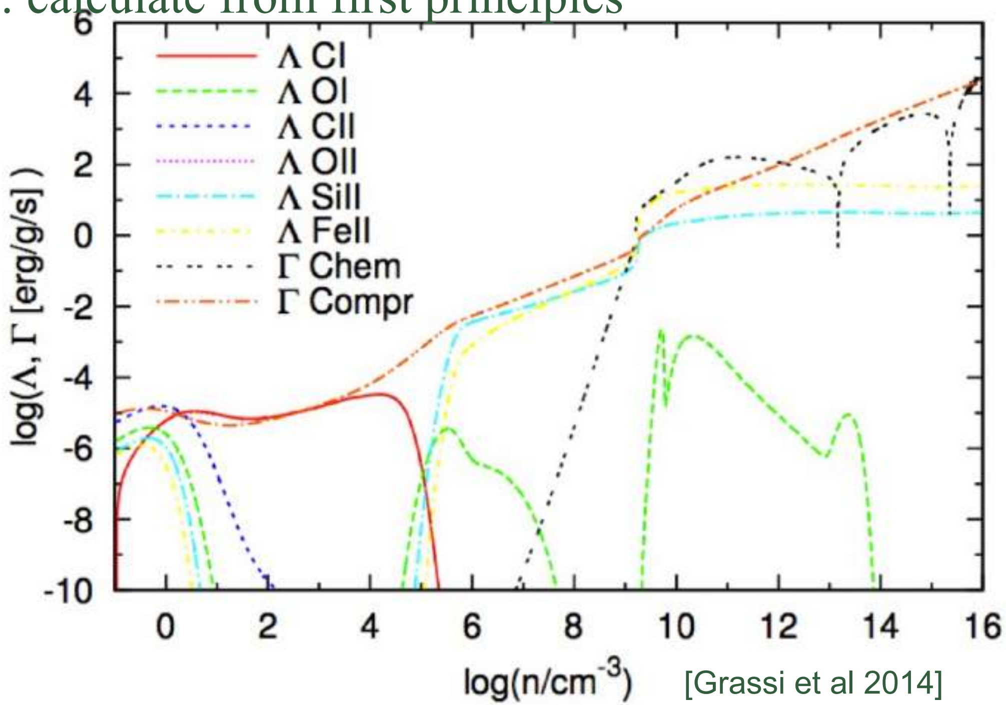
[Dalgarno & McCray 1972]

Numerical Implementation III - Cooling

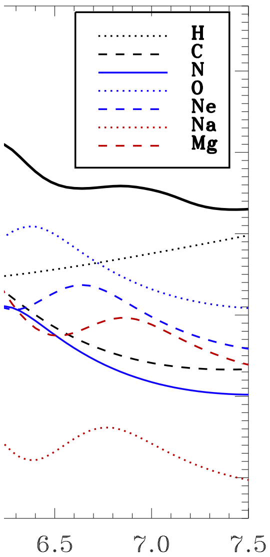
- The standard approach for cooling in the interstellar medium is to use a table lookup, and assume that the cooling rates (per H atom)[2] is a function of temperature alone
- A more sophisticated approach is to have one table per species
- Even better: calculate from first principles



[Dalgarno & McCra



[Grassi et al 2014]

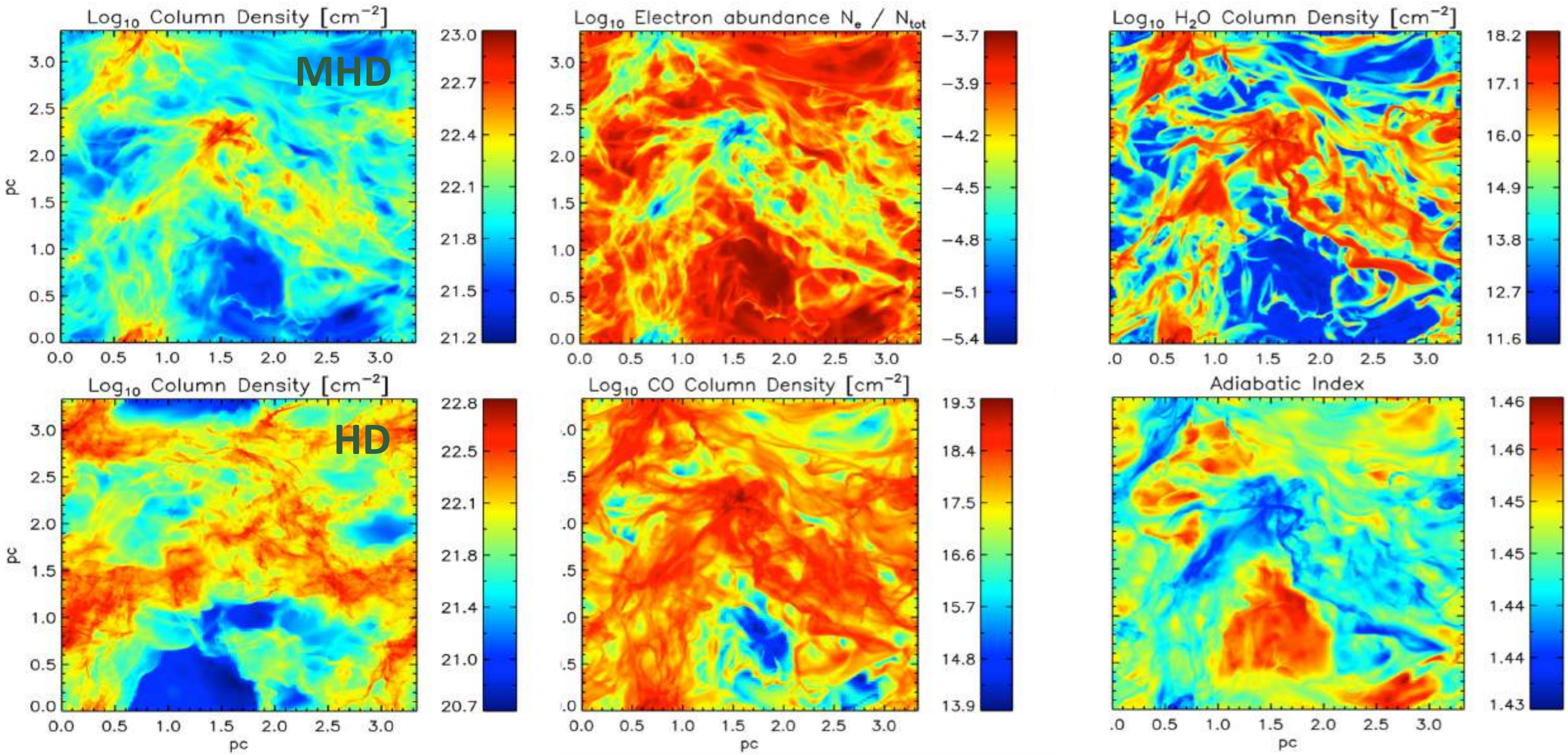


[Shure 2009]

Summary of microphysics

- Thermal processes and ***chemistry*** are important for the physical structure of both the ISM and protoplanetary systems
- Cooling rates, ionization fraction, and magnetic resistivity all depend on the ***chemical composition***, which in turn depends on radiation transport and dynamical effects such as dissipation and compressional heating/cooling
- Typically, in numerical codes cooling and heating is based on simple fitting formulas (heating) & table lookups (cooling), and maybe radiative transfer.
- The drive to deliver direct predictions for observations and quantitative models of star formation have led several groups to develop and integrate ***detailed chemical models*** to couple gas, magnetic fields and radiation
- **KROME** (kromepackage.org), partly developed at NBI, is one of the most complete astrochemistry packages.

Turbulent Molecular Cloud – 42 species, 500 reactions



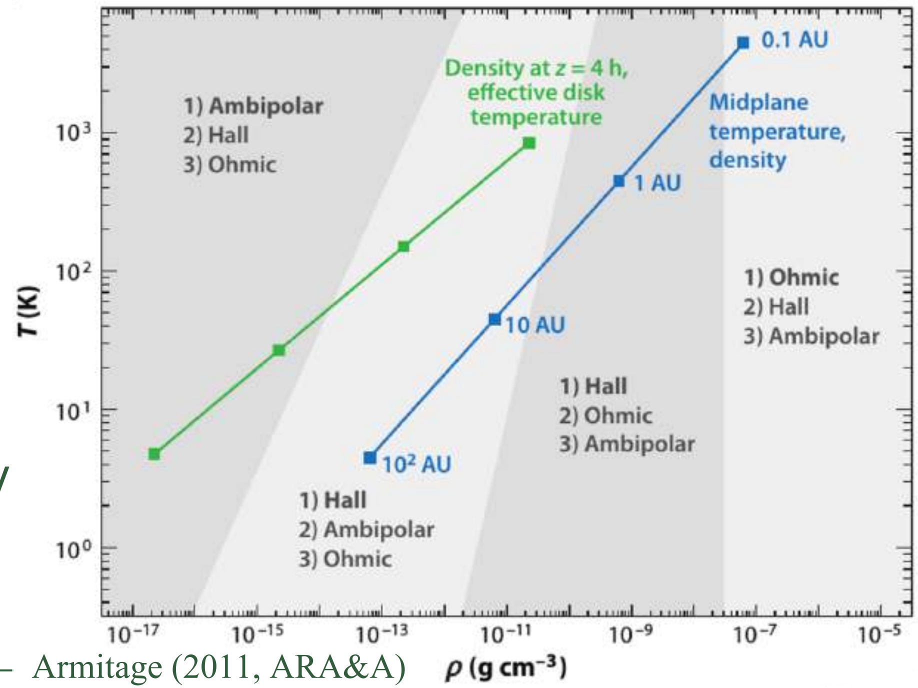
- Large diff. in HD & MHD;
- ISM is magnetized;
- Affects SFR, IMF;

- Most H molecular;
- CO effectively formed;
- Free ions even @ 10-50K;

- Only small changes in γ.

Modern microphysics: "Non-ideal" MHD

- A good chemical description of the gas is crucial to provide a correct description of the number of free electrons, and therefore the ionization fraction. Poor mans alternative is with tables like for cooling.
- ***Ambipolar diffusion*** can lead to “leaking” of magnetic flux and conduction of heat during protostellar collapse, which has implications for the formation of disks.
- ***The Hall term*** is important in protoplanetary disks, particularly at intermediate densities (i.e., larger radii).
- ***Ohmic resistivity*** and heating is likely important in the inner regions of protoplanetary disks (i.e., higher densities).
- Non-ideal magnetic effects are currently a very active area of research (both here at NBI and elsewhere).

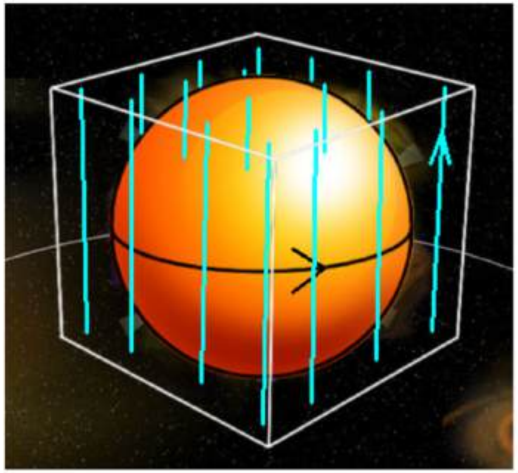


Armitage (2011, ARA&A)

An example: ambipolar and ohmic diffusion in 3D simulations of star formation

Initial conditions

- Spherical cloud with mass: 1 $M_\odot$
- Radius: 2500 AU
- Uniform density + 10% $m = 2$ perturbation
- Temperature: 10 K
- Solid body rotation (1%)
- Vertical B field: $\mu = 4$



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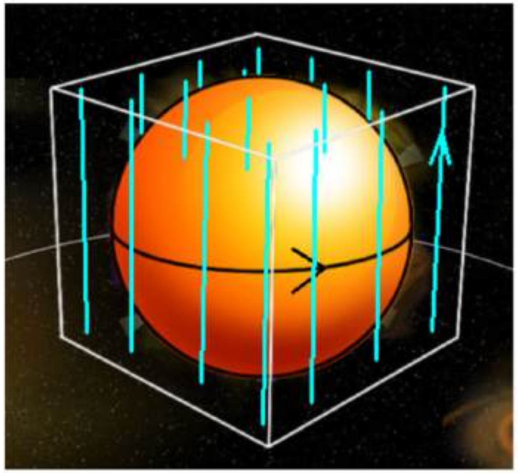

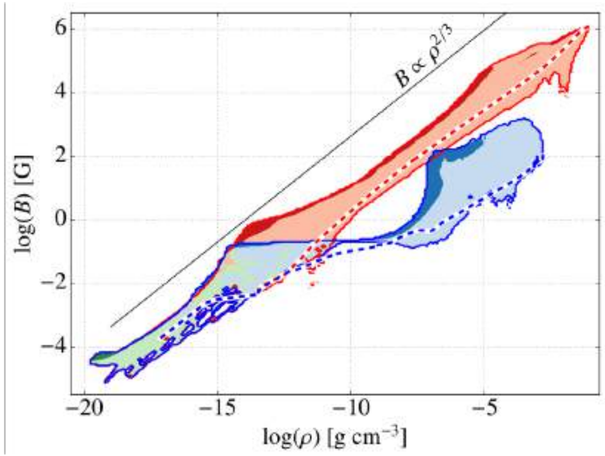

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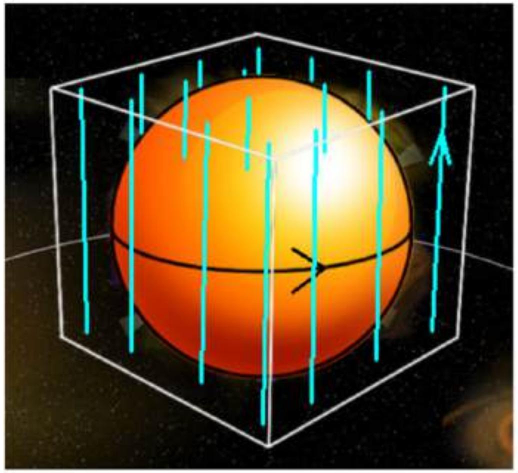

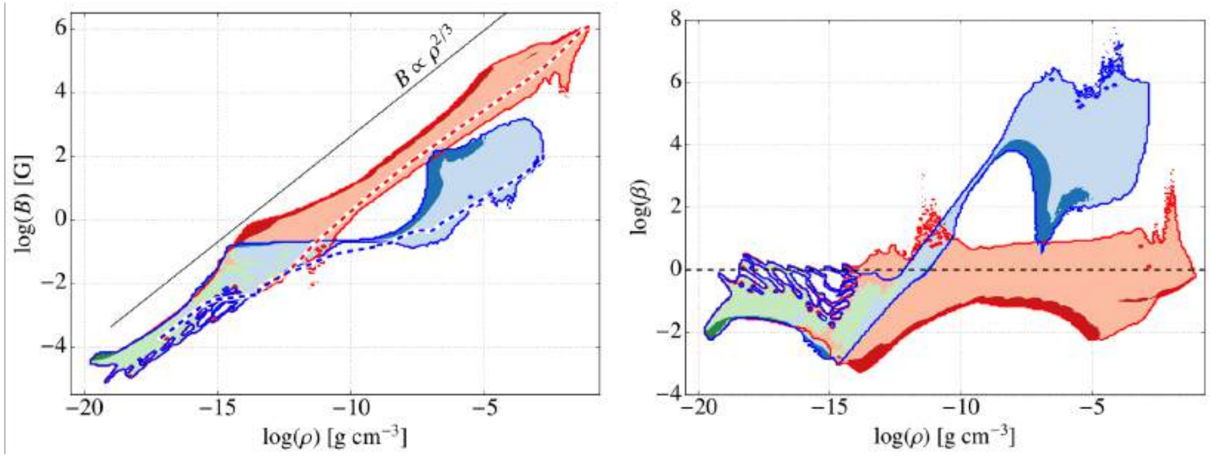

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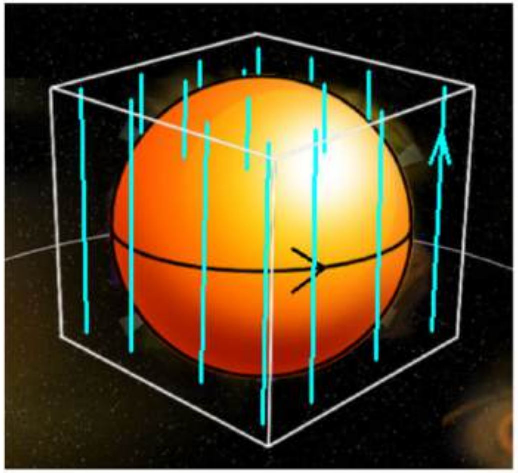

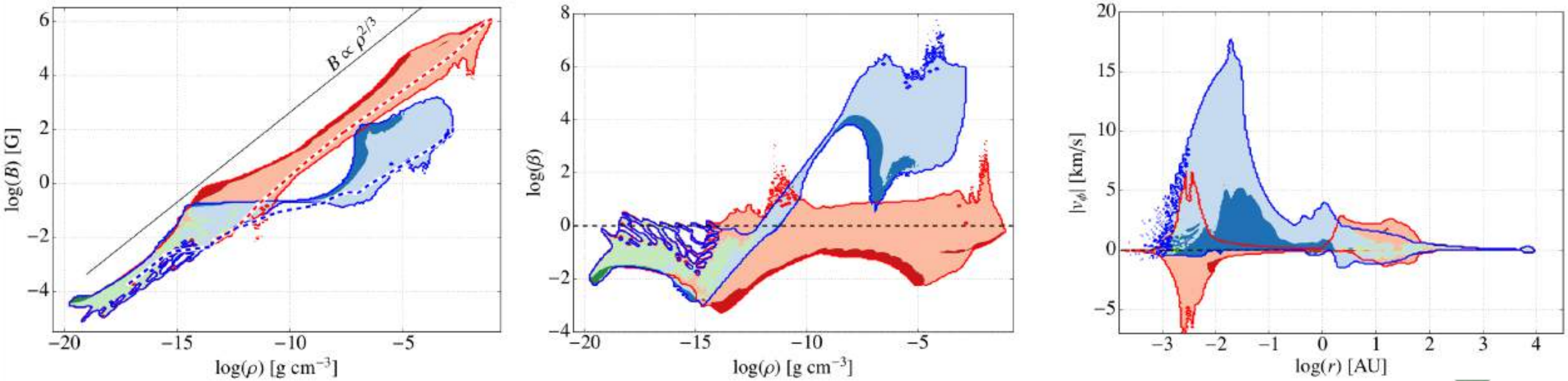

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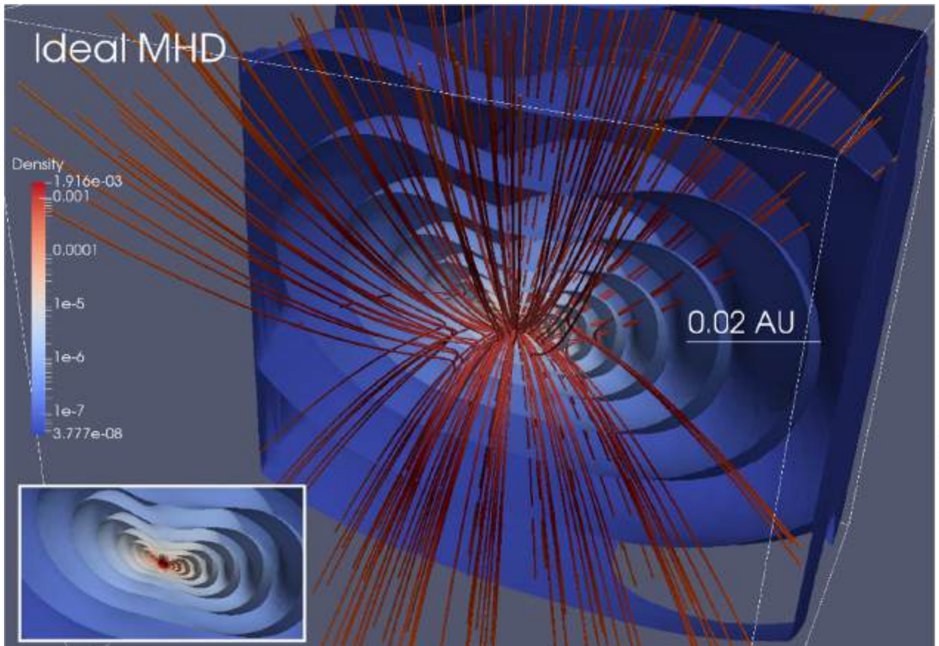
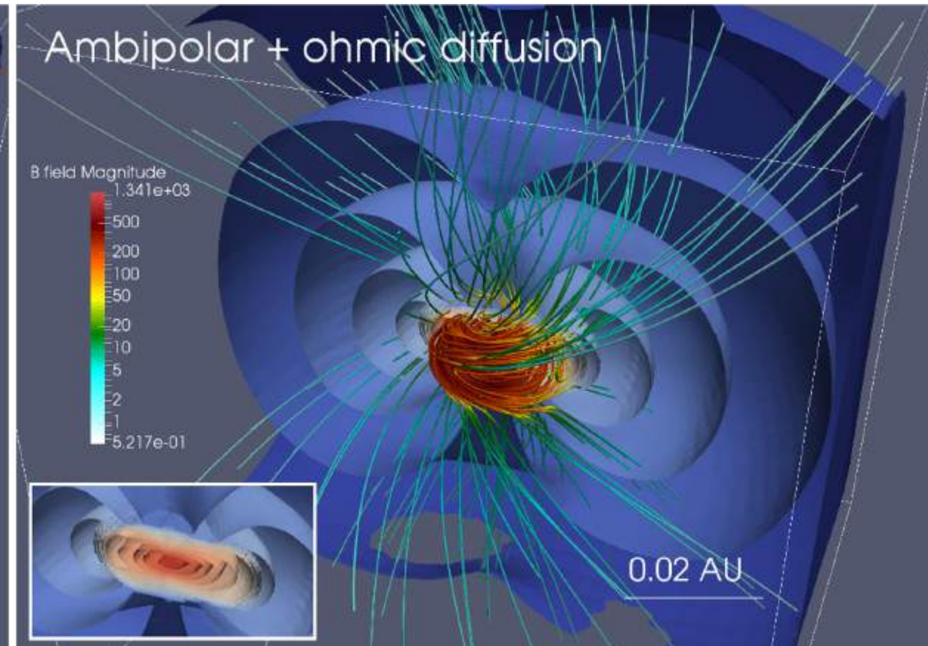
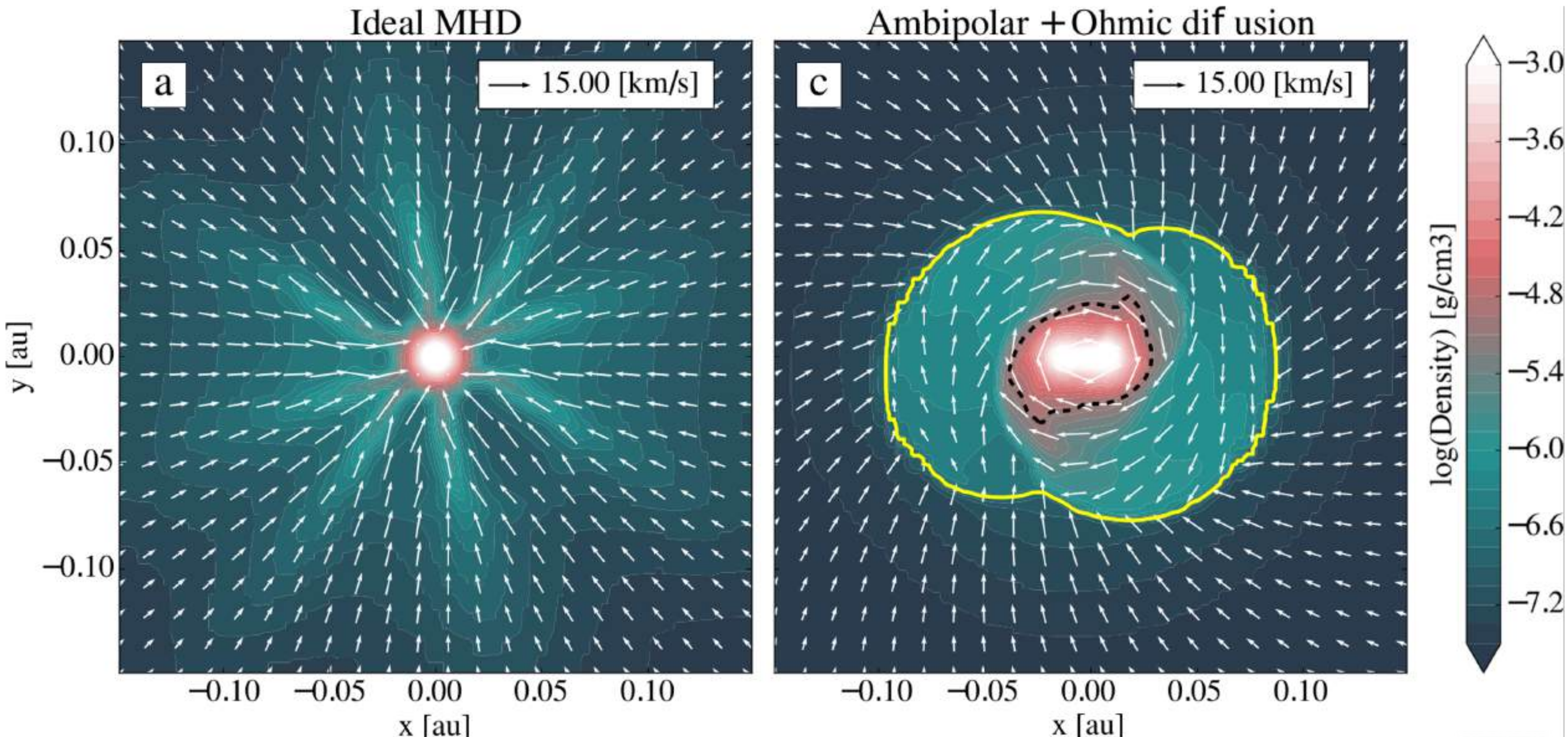




An example: ambipolar and ohmic diffusion in 3D simulations of star formation



Electromagnetic Sources and non-ideal MHD

In the second week we looked at fluid dynamics. Today we'll look at sources

Resistivity and Ohmic heating:

- Ohmic heating is Ohm's law for plasmas. High current→high T
- A plasma is resistive due to collisions between electrons, ions and neutrals
- Important at high densities and low degrees of ionization

Constraints:

Fluid viscosity

$$\mathbf{S}_{mom} = -\rho\nabla\phi + \mathbf{T}_{stress}$$

$$S_{energy} = Q_{stress} + Q_B - \nabla\cdot\mathbf{q} + Q_{heating} - \Lambda_{cooling}$$

$$\nabla^2\phi = 4\pi G\rho$$

Gravity

$$\mathbf{E} = -\mathbf{u}\times\mathbf{B} + \eta\mathbf{J} + \frac{\mathbf{J}\times\mathbf{B}}{qn}, \quad \mathbf{J} = \nabla\times\mathbf{B}$$

$$Q_B = \mathbf{E}\cdot\mathbf{J} = \eta\mathbf{J}^2, \quad q_B = -\boldsymbol{\kappa}_{BB}\cdot\nabla T$$

Resistivity and Ohmic heating

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Hall Effect:

- Happens when ions and dust particles decouple from the magnetic field, and instead couple to neutrals

- This can be seen by rewriting

$J/qn = u_i - u_e \rightarrow -u \times B + J/qn \times B = u_e \times B$

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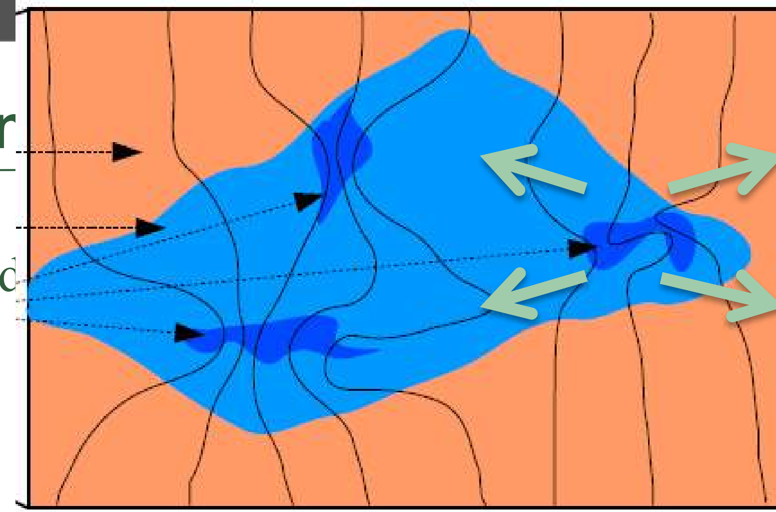
Electromagnetic Sources ar



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Ambipolar Diffusion:

- Is important in molecular cores and at the edge of PP disks, where ions drift through neutrals
- Conducts heat efficiently due to collisions between the species, but anisotropically, mostly along field lines ($\kappa_{\parallel} \gg \kappa_{\perp}$)
- Allows flux to diffuse with ions

$$S_{energy} = Q_{stress} + Q_B - \nabla \cdot \mathbf{q} + Q_{heating} - \Lambda_{cooling}$$

$$\nabla^2 \phi = 4\pi G \rho$$

Gravity

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Hall Effect

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Resistivity and Ohmic heating

Ambipolar diffusion

Summary: Electromagnetic Interaction

- A good chemical description of the gas is crucial for a correct description of the ionization fraction, and the number of free electrons
- Ambipolar diffusion plays and important role at lower densities, in molecular cloud cores and the outskirts of protoplanetary disks
- Ambipolar diffusion can help in leaking magnetic flux during and conduct heat during the protostellar collapse
- The Hall effect may be important at intermediate densities (~10-50 AU) in protostellar disks
- Ohmic resistivity and heating may play a role in the inner regions of a protoplanetary disk
- Non-ideal MHD is a very active research area both internationally and at the NBI