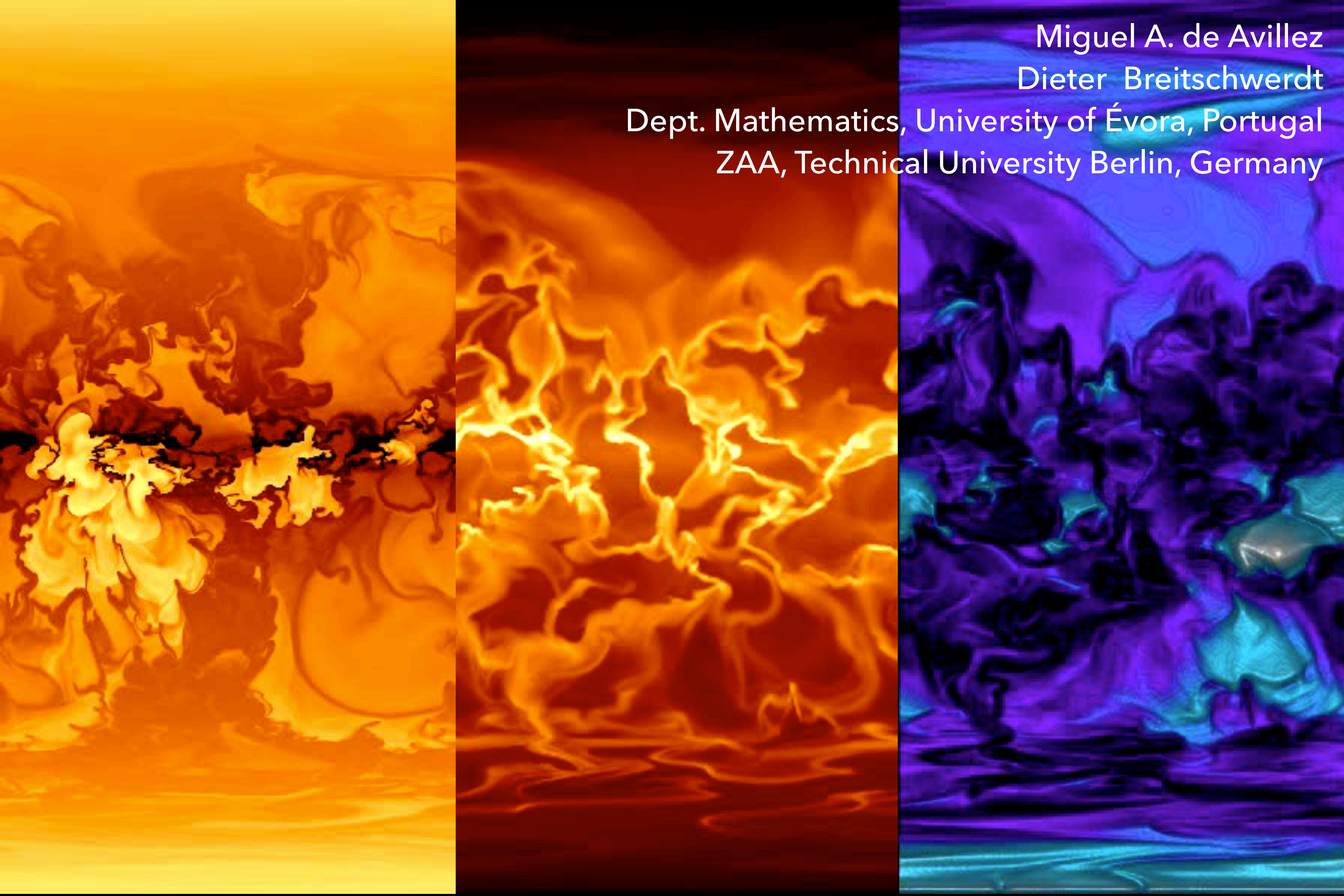

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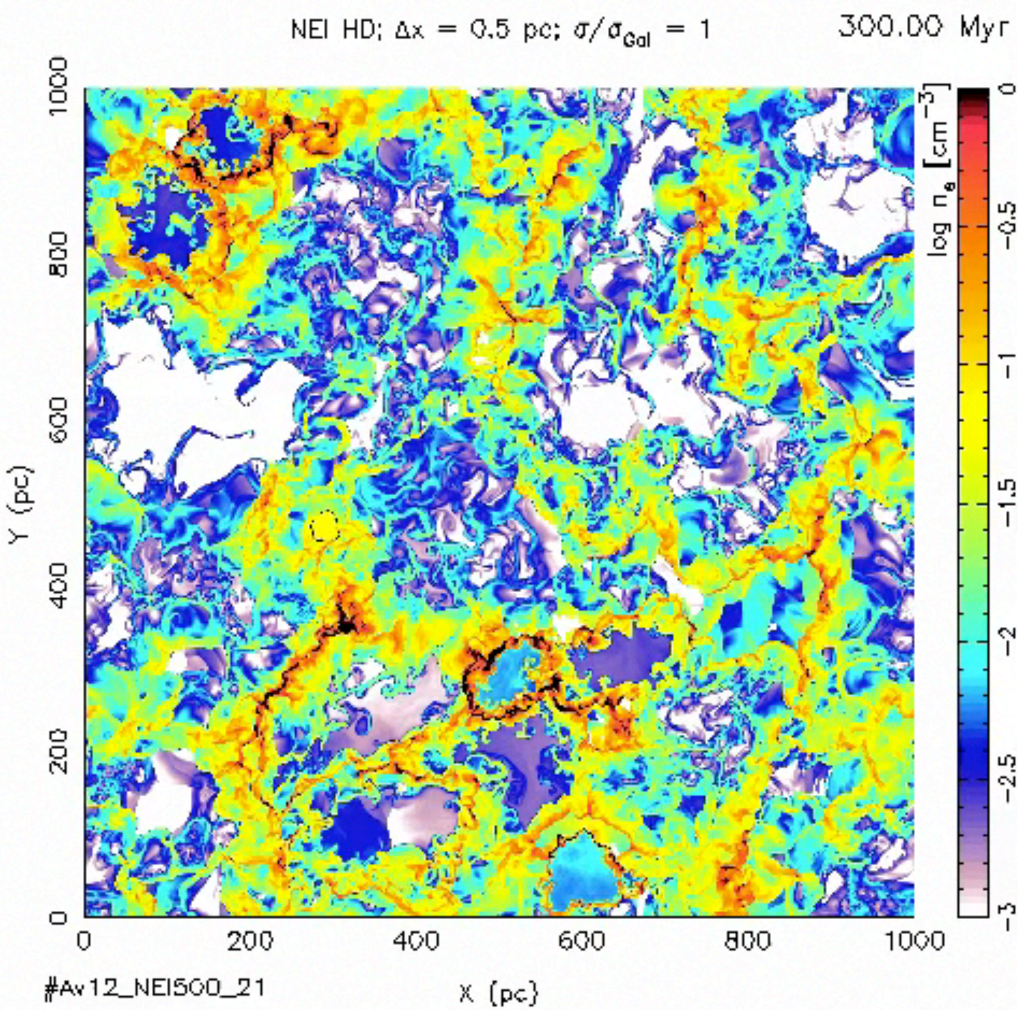
# The Importance of the Atomic History in Time-Dependent Simulations of the Interstellar Gas

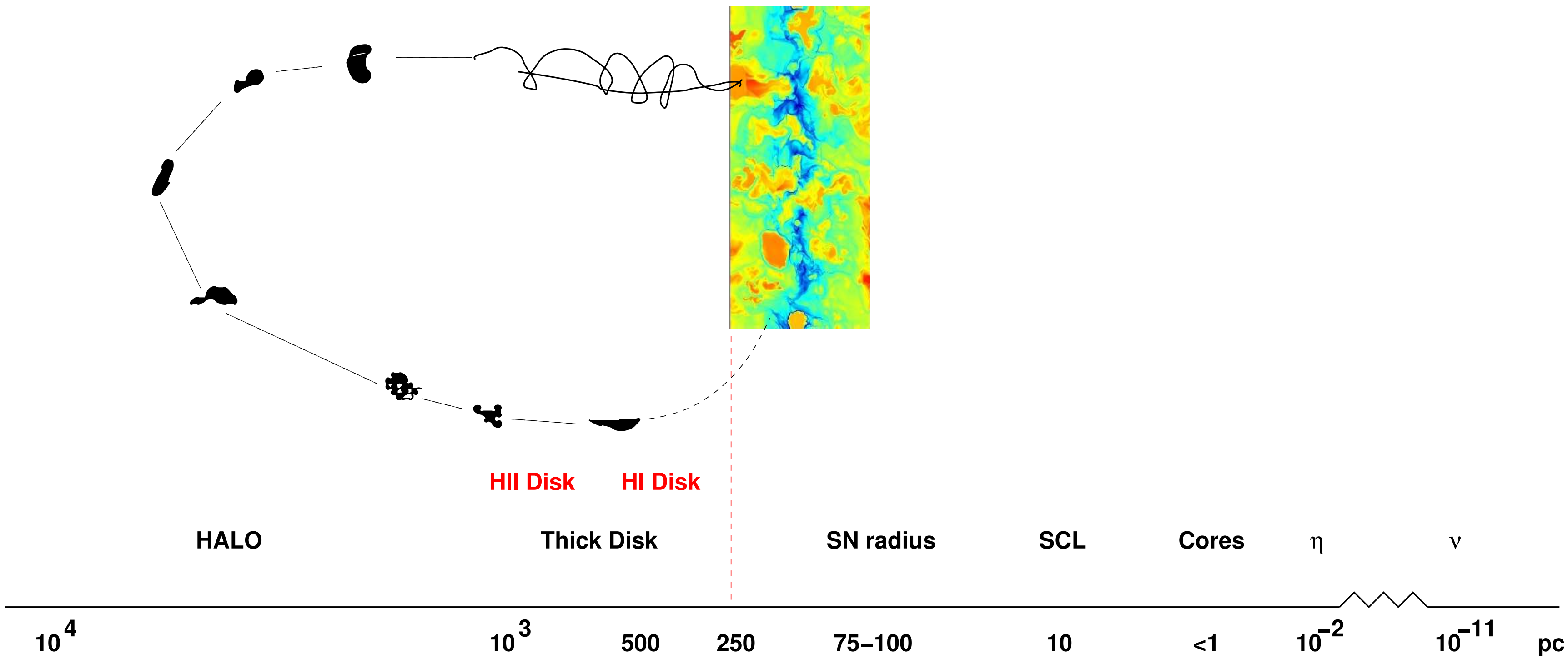
Parallel AMR
Coarse resolution = 8 pc
Higher resolution = 0.5 pc
Effective grids of $2000^3$ cells
Evolution time = 500 Myr
Cut through the Galactic midplane

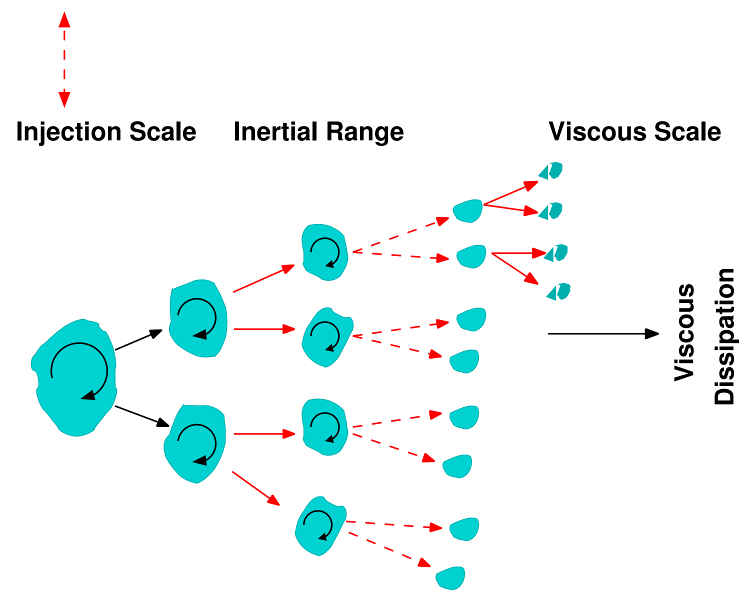



- → Ionizing
- → Recombining
- → Cooling
- → Turbulent mixing
- → Conductive interfaces
- → Particles acceleration (DSA)

← FREE ELECTRONS DISTRIBUTION

- → Non-equilibrium plasmas
- → Thermal + Non-thermal
- → Feedback


HII Disk
HI Disk
HALO
Thick Disk
SN radius
SCL
Cores
η
ν
10 4
10 3
500
250
75–100
10
<1
10–2
10–11
pc


Injection Scale
Inertial Range
Viscous Scale
Viscous Dissipation

Thermal translational energy

Energy stored in (or delivered) from high ionization stages

Energy stored in (or delivered) from excited states

$$\rho e = \frac{3}{2}(n_{tot} + n_e)k_B T + \sum_Z \sum_{z=1}^{Z} n_{Z,z} \left( \sum_{l=0}^{z-1} \Phi_{Z,l} \right) + \sum_Z \sum_{z=1}^{Z} \left[ \sum_{j=n_o+1} n_{Z,z,j} \left(\Delta E_{j,n_o}\right)_{Z,z} \right]$$

Total energy loss (gain) is not synchronized with equivalent decrease (increase) of temperature.

$$P - \rho \left( \sum_{Z,z} \frac{n_{Z,z}}{\rho} + \frac{n_e}{\rho} \right) k_B T = 0$$

Feed into the momentum equation

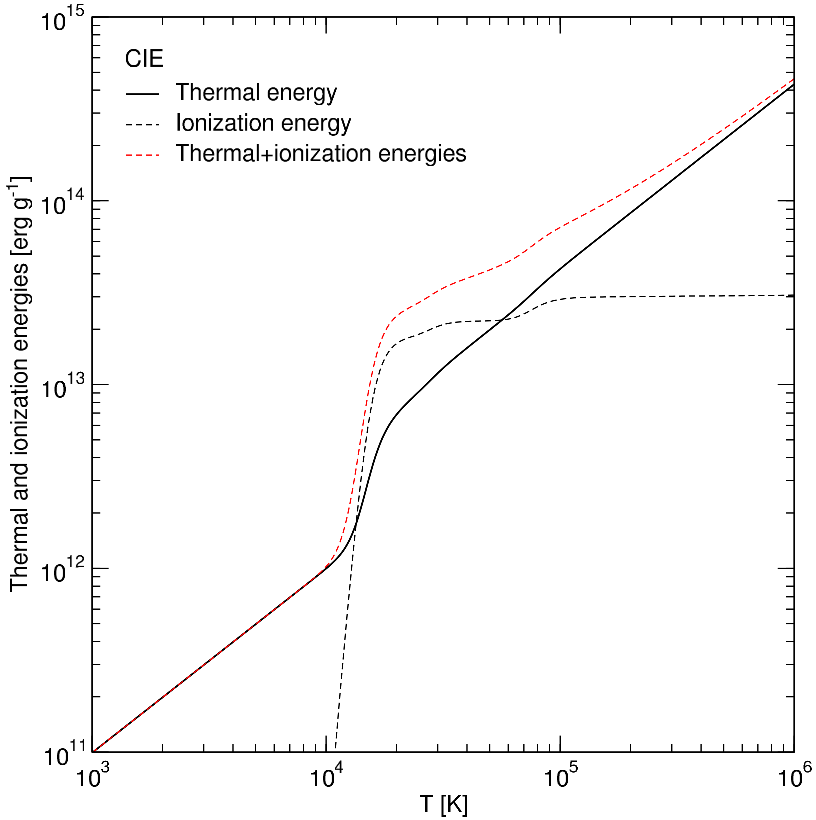
Affects the dynamics

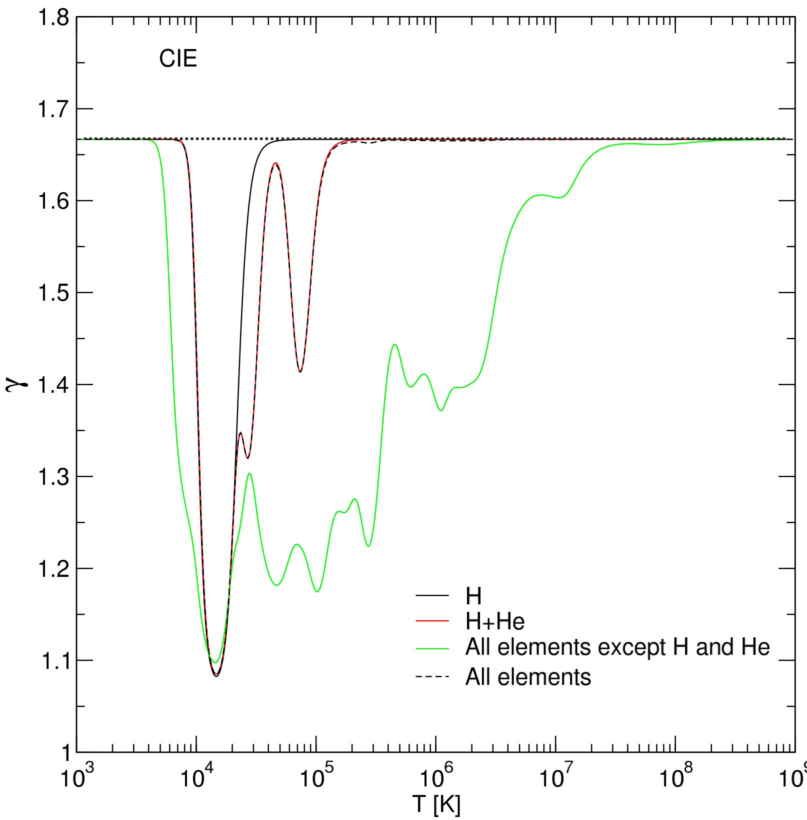
$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v} + P_{th}) = -\rho g + S_{\rho \vec{v}}$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot [(\rho e + P_{th})\, \vec{v}] = \rho \vec{v} \cdot \vec{g} + \nabla \cdot (\kappa \nabla T) + \Gamma_{SN} + \mathcal{H} - n_e n_H \Lambda(T)$$

$$\rho u = \frac{3}{2}(n_{tot} + n_e)k_B T + \sum_Z \sum_{z=1}^{Z} n_{Z,z} \left( \sum_{l=0}^{z-1} \Phi_{Z,l} \right) + \sum_Z \sum_{z=1}^{Z} \left[ \sum_{j=n_o+1} n_{Z,z,j} \left( \Delta E_{j,n_o} \right)_{Z,z} \right]$$

$$\gamma = \frac{c_p}{c_v}$$

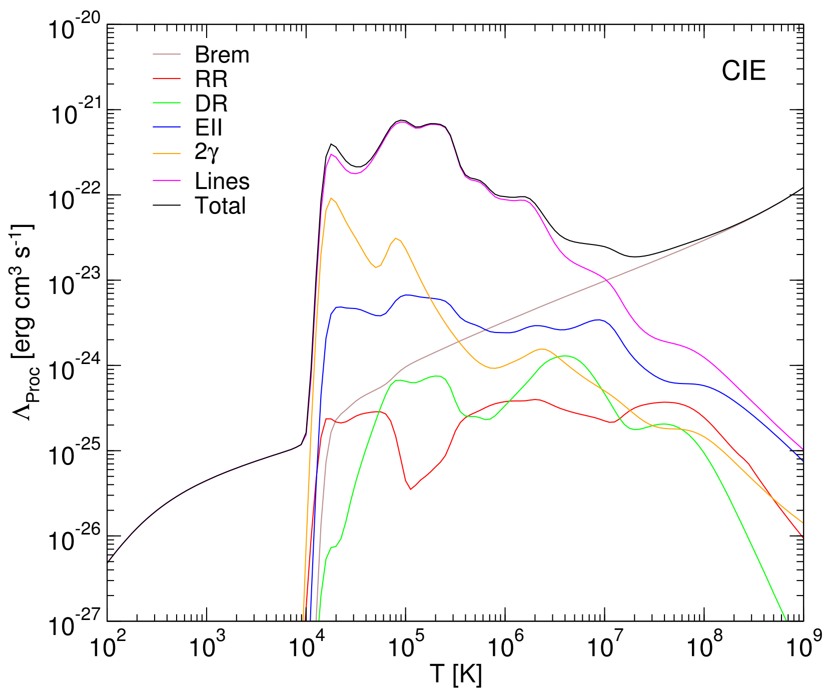


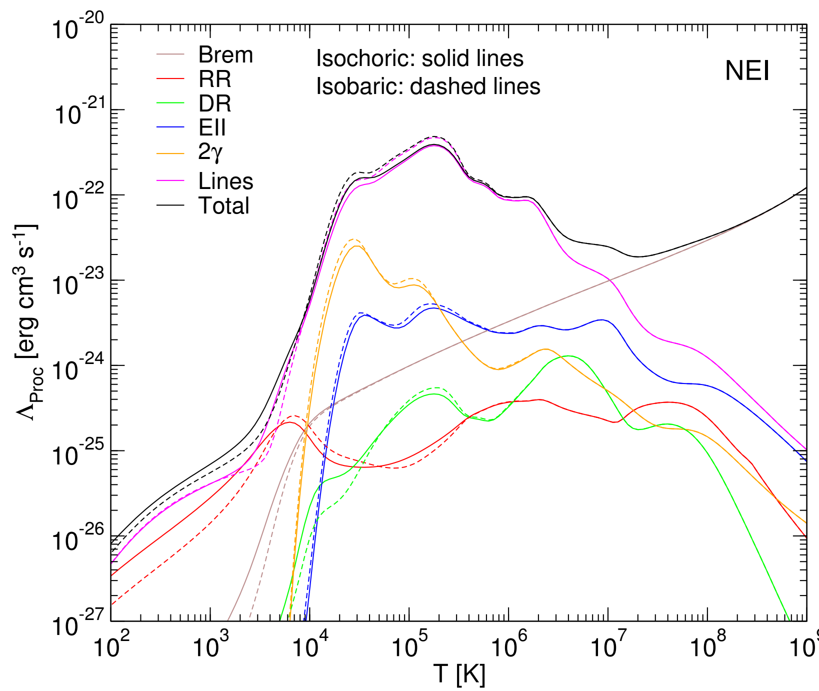



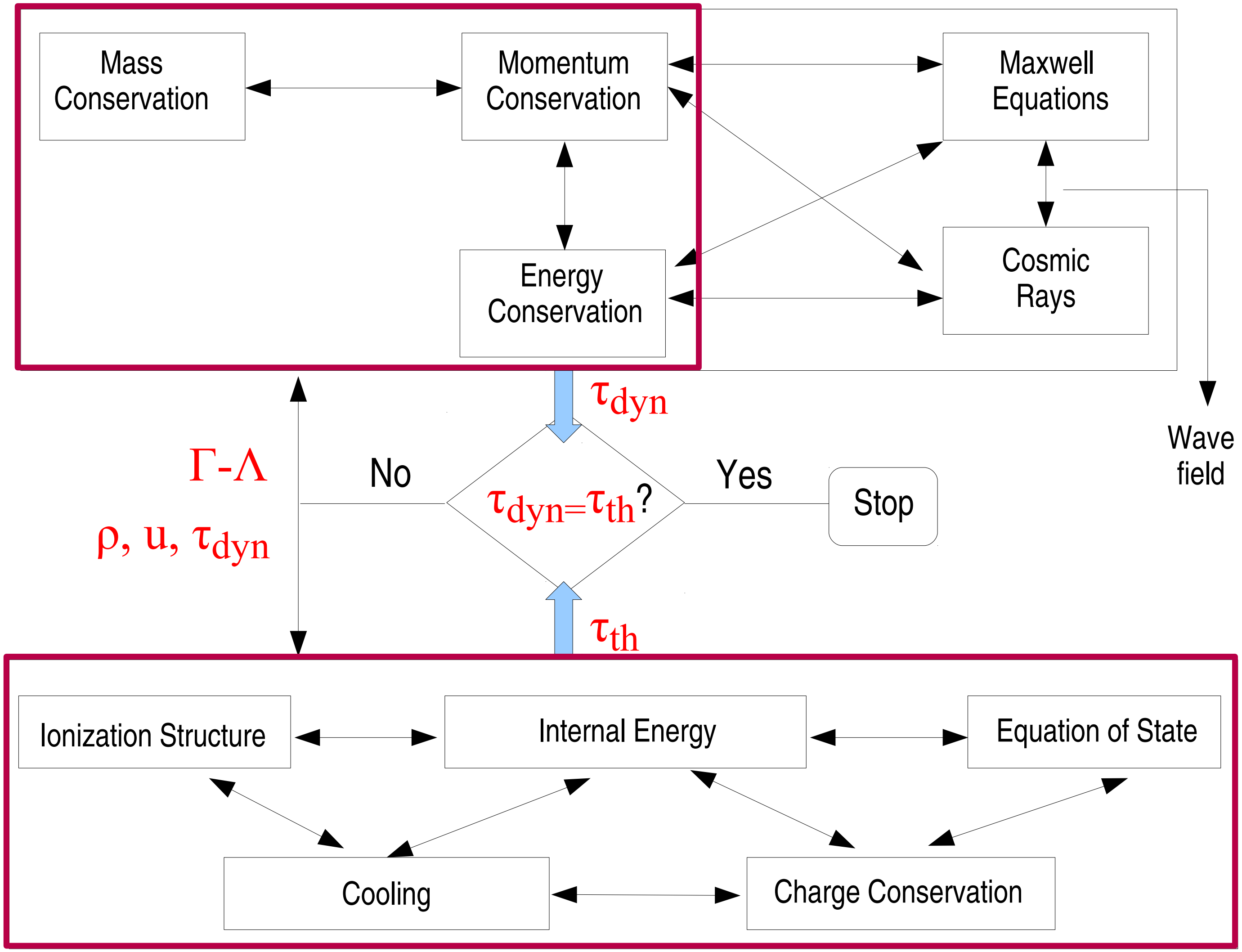
- Maxwell-Boltzmann distribution
- Temperature equilibration ions and electrons
- Include a fixed cooling function (of a gas parcel)
- Adiabatic parameter constant (5/3)
- Internal energy includes only the thermal component
- Neglect the feedback of dynamics

→ All fluid elements have the same atomic history

→ Not correct






$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_\rho$$

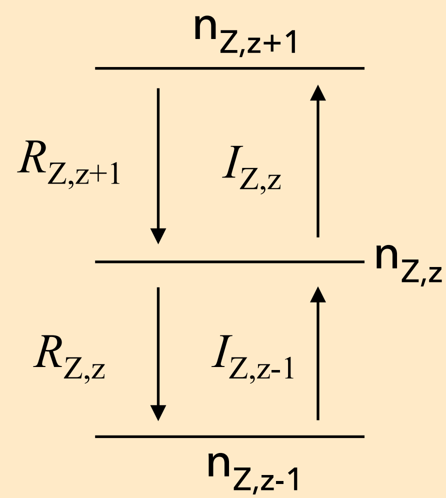
$$\frac{\partial \rho X_{Z,z}}{\partial t} + \nabla \cdot (\rho X_{Z,z} \vec{v}) = \rho S_{Z,z}$$

$$\frac{d\,n_{Z,z}}{dt} = I_{Z,z-1} n_{Z,z-1} - \left(I_{Z,z} + R_{Z,z}\right) n_{Z,z} + R_{Z,z+1} n_{Z,z+1}$$

$$R_{Z,z} = n_e \left(\alpha^{rr}_{Z,z} + \alpha^{dr}_{Z,z}\right) + \sum_{\tilde{Z},\tilde{z}} \alpha^{ce}_{\tilde{Z},\tilde{z}} \tilde{n}_{\tilde{Z},\tilde{z}}$$

$$I_{Z,z} = \zeta_{Z,z} + n_e \left(C^{eii}_{Z,z} + C^{ea}_{Z,z}\right) + \sum_{\tilde{Z},\tilde{z}} C^{ce}_{\tilde{Z},\tilde{z}} \tilde{n}_{\tilde{Z},\tilde{z}}$$

$$\zeta_{Z,z} = \zeta^{ph}_{Z,z} + \zeta^{c}_{Z,z} + \zeta^{pe}_{Z,z}$$




$$\frac{d\,n_{Z,z,j}}{dt} = \sum_{m<j} Exc_{m\to j} + \sum_{n>j} Dexc_{n\to j} - \sum_{j>m} Dexc_{j\to m} - \sum_{j<n} Exc_{j\to n}$$

$$\frac{d\,n_{Z,z,j}}{dt} = \sum_{m<j} C^{e,X}_{mj} n_X n_{Z,z,m} + \sum_{n>j} \left(C^{d,X}_{nj} n_X + A_{nj}\right) n_{Z,z,n}$$

$$- \sum_{j>m} \left(C^{d,X}_{jm} n_X + A_{jm}\right) n_{Z,z,j} - \sum_{j<n} C^{e,X}_{jn} n_X n_{Z,z,j}$$

- ➔ Non-equilibrium ionization: H, He, C, N, O, Ne, Mg, Si, S, Ar, Fe + H, C, O chemistry
- ➔ 70-level ions
- ➔ Abundances (solar and pre-solar)
- ➔ Equal and/or different temperature for electrons and ions
- ➔ Thermal and non-thermal particle distributions (e.g., kappa, n, cosmic rays)

- ➔ Electron impact ionization (total and shell), inner-shell excitation auto-ionization
- ➔ Radiative (RR) and dielectronic (DR) recombination followed by cascades
- ➔ Charge-transfer reactions
- ➔ Photoionisation + Auger photoelectrons + Secondaries
- ➔ Continuum (bremsstrahlung, free–bound, two-photon)
- ➔ Line (permitted, semi-forbidden, forbidden) emission

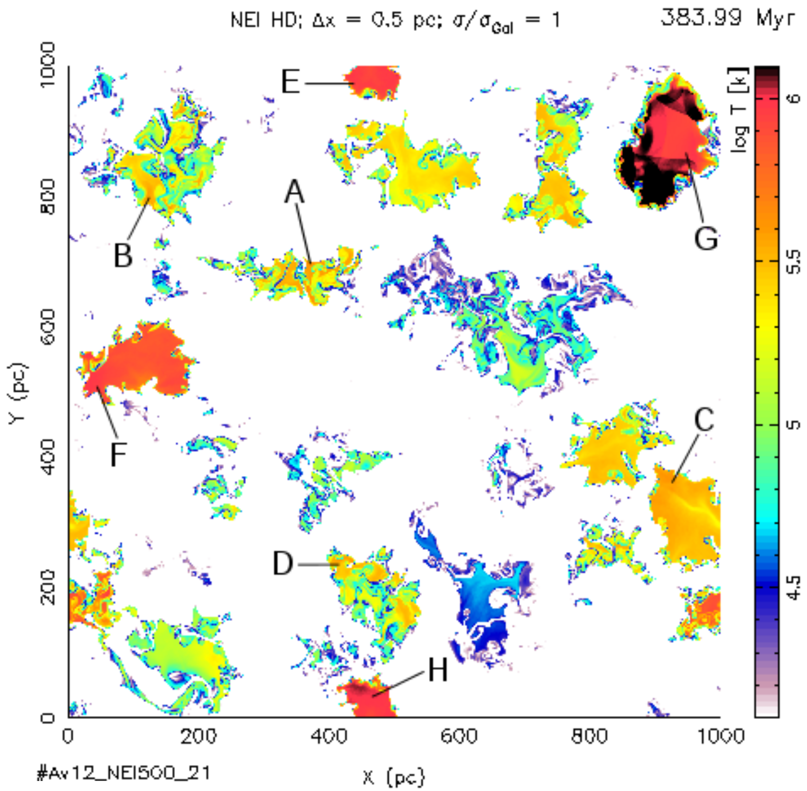
- ➔ Rates calculated from cross sections on the fly
- ➔ Excitation/deexcitation rates calculated from collision strengths (R-Matrix calculations)
- ➔ Calculations are made in accelerators/coprocessors while CPUs are idle for $10^{-5}$ s
- ➔ Parallel computing - dynamical model in CPUs + thermal model in GPUs/Xeon Phi

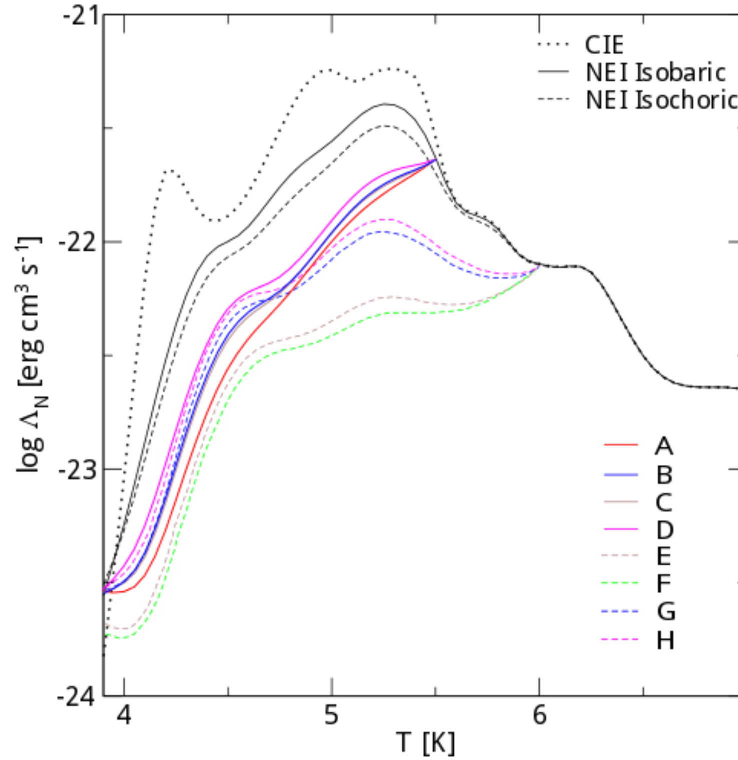
- 3D multi-fluid HD or MHD evolution over 500 Myr
- Grid: 1 kpc × 1kpc × ± 15 kpc   Δx=0.25 pc and 0.5 pc ($4000^3$ cells per $kpc^3$)
- Density distribution from observations (Dickey & Lockman 91, Ferriere 98)
- Star Formation based on thresholds: $n > 100\ cm^{-3}$ & $T<100$ K
- Formation (5% efficiency) from core fragmentation of MCs
- IMF for stars with 7-60 solar masses (Fuchs et al. 2006)
- Trace motion of OB stars ($v_{rms}$~5 km/s) and main-sequence time evolution
- SNe types Ib+c and II: random + clustered (~60%) + yields
  - Rate: $1.9 \times 10^{-2}\ yr^{-1}$ (Diehl et al. 2006; Cappellaro et al. 1999)

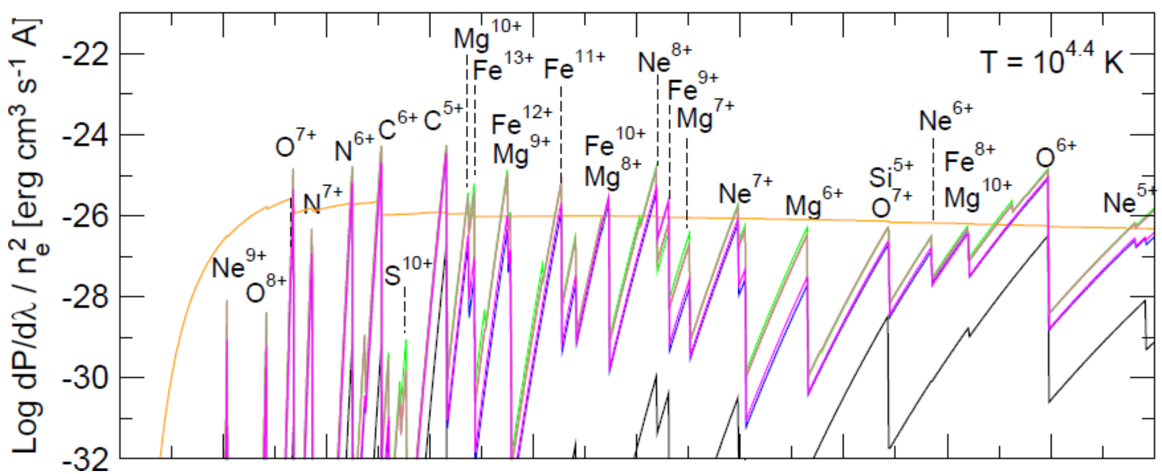
    26.9 $Kpc^{-2}\ Myr^{-1}$ in a Galactic disk with R=15 kpc
- SNE type Ia randomly distributed with $h_z$=325 pc (Freeman 1987)
  - Rate: $4 \times 10^{-3}\ yr^{-1}$ (Cappellaro et al. 1999; see also Ferriere 2001)

    5.7 $Kpc.^{-2}\ Myr^{-1}$ in a Galactic disk with R=15 kpc

- ➔ Background heating due to diffuse UV photon field calculated from the stars
- ➔ Galactic gravitational field by stars (Kuijken & Gilmore 1989) + self gravity
- ➔ Heat conduction (Dalton & Balbus 1993)
- ➔ Magnetic field (random + mean components 6 μG)



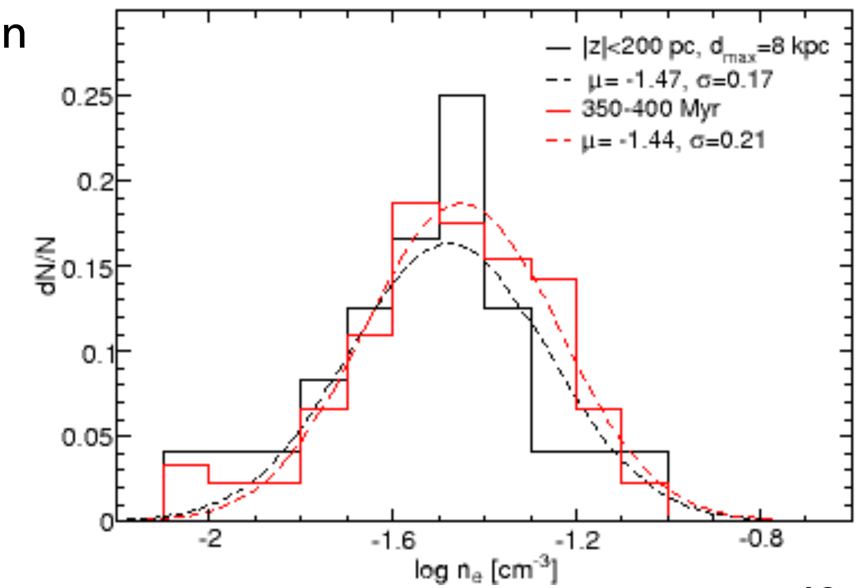




Avillez+Breitschwerdt (2012)

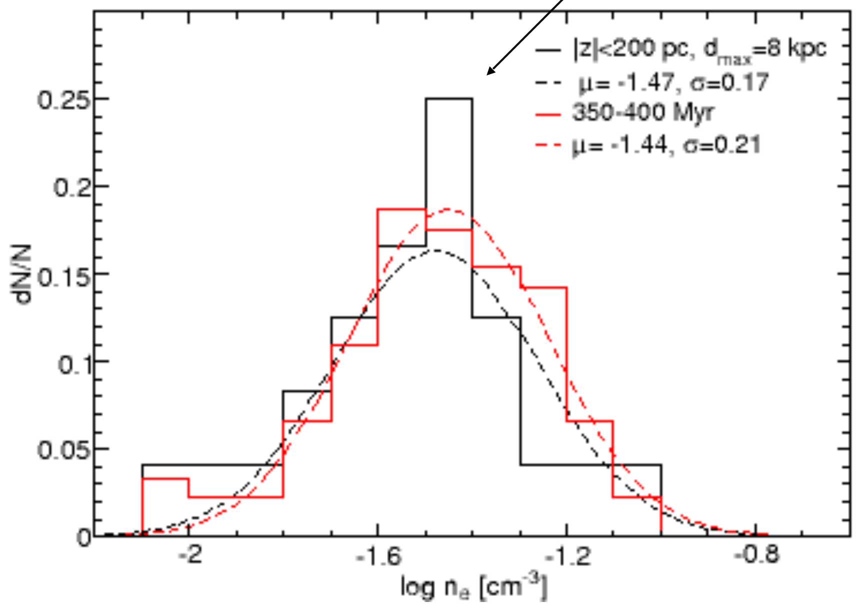
- ➡ Jenkins (2013): FUSE observations of UV spectra of 44 hot subdwarf stars a few hundred parsecs away from the Sun
  - ✓ Compare column densities of ArI to those go OI
  - ✓ The measured deficiency [ArI/OI]=-0.427 below the expectation for a fully neutral medium
  - ✓ Implies that the electron density $n_e$~0.04 $cm^{-3}$ if n(H)=0.5 $cm^{-3}$

- ➡ Dispersion measurements against pulsars of known distances (Berkhuijsen+ 2008; Gaensler+ 2008; Schnitzeler 2012, see also Avillez+2012):
  - ✓ Electrons have a clumpy distribution
  - ✓ Log $n_e$ has a Gaussian PDF
  - ✓ $n_e$ (z=0 pc)=0.02-0.04 $cm^{-3}$

$$\log \langle n_e \rangle = -1.47 \pm 0.02$$ $n_e$~0.033 $cm^{-3}$



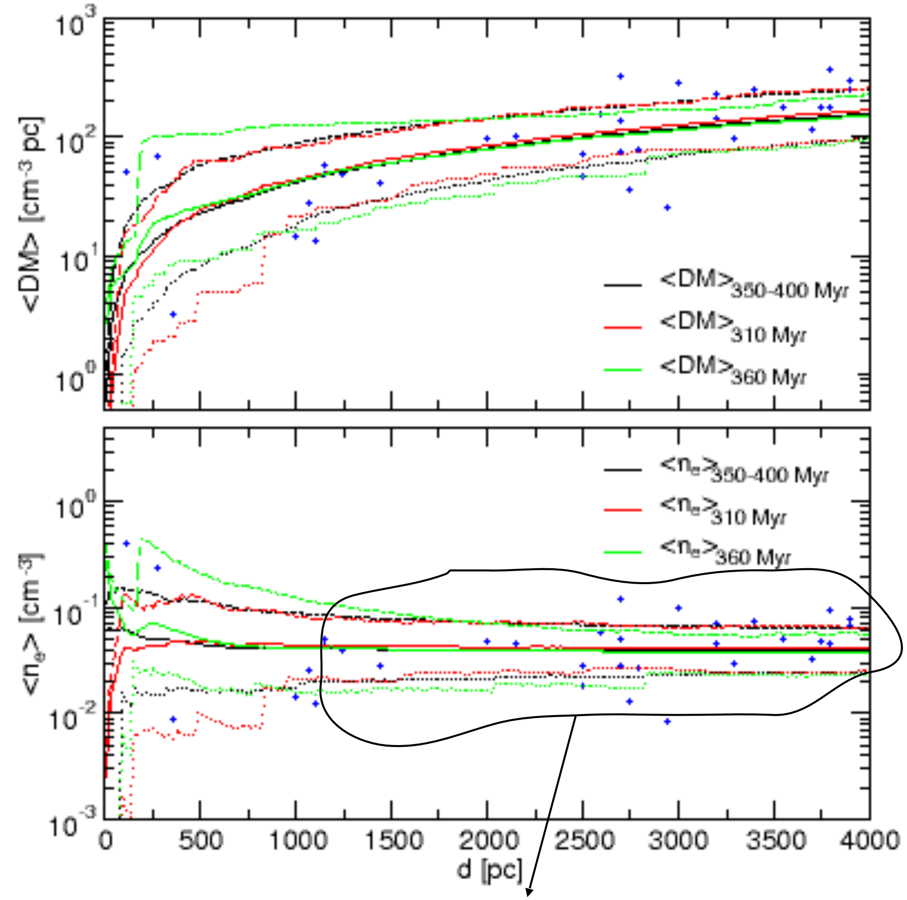
From pulsars DMs up to 8 kpc from Sun




33 pulsars at |z|<200 pc with reliable distance estimates.

$$\log \langle n_e \rangle = -1.47 \pm 0.02$$

$n_e \sim 0.033\ cm^{-3}$




Dispersion is constant with d

Electrons: clumpy distribution.

Avillez+ 2012, 2019

- Cooling time < Recombination time of ions
- Plasma keeps a record of its history - Need to include all the ions
- The ionization structure varies in space and time and depends on the ICs
- The cooling paths can be quite different for plasmas with the same initial temperature, but having different evolution histories;

- Full blown simulations imply ten most abundant elements (112 ions), thermal and non-thermal electron/proton distributions, large database of cross sections and collision strengths.
- CRs ISM simulations must include DSA and full calculation of ionisation, recombination and excitation/deexcitation rates using cross sections and the local electron/proton distribution function

**HD/MHD/CR-MHD + ATOMIC/MOLECULAR PHYSICS**


"That's all Folks!"