ISM in Silico

Pierre Lesaffre

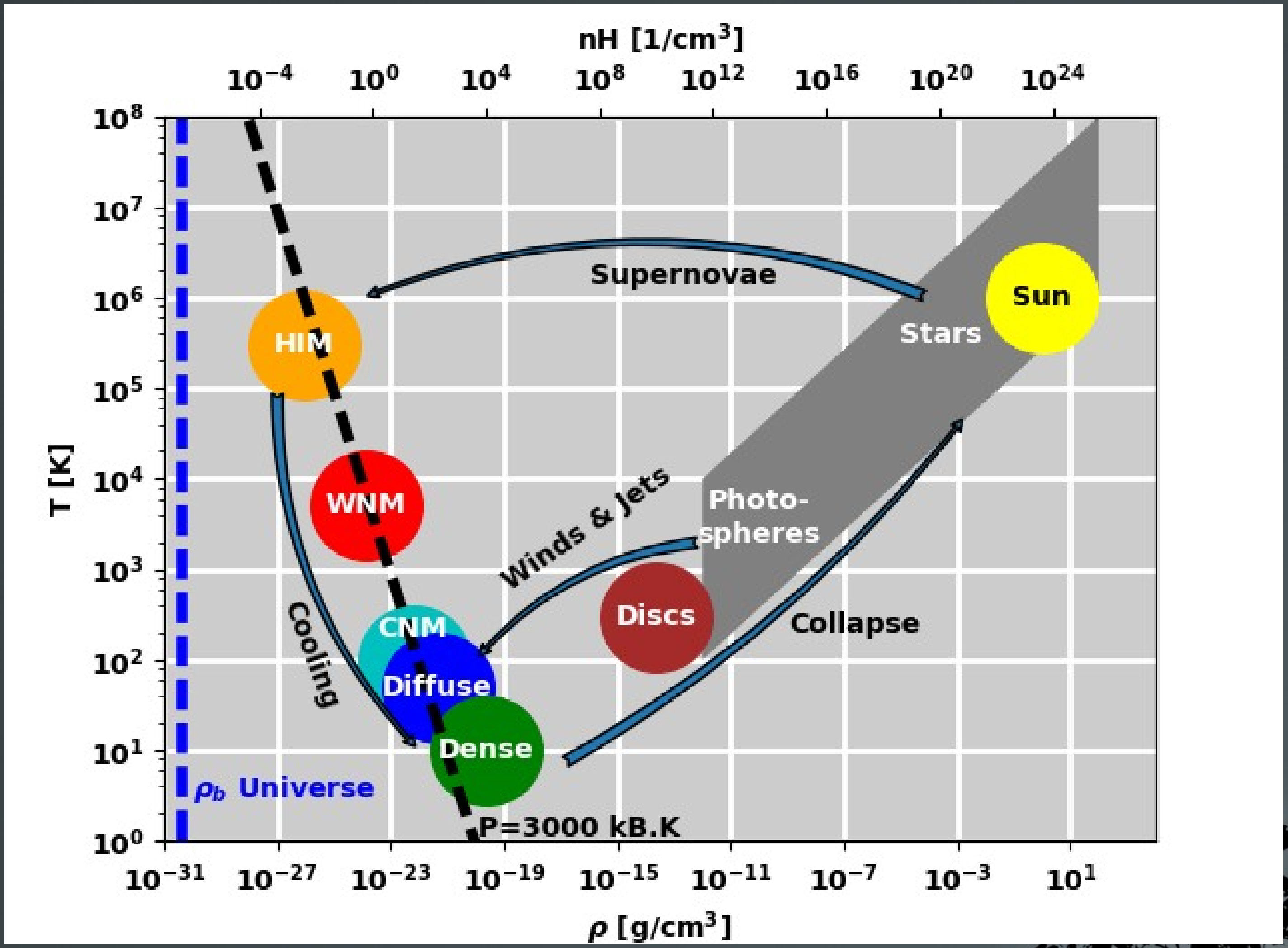
Thanks:

A. Faure, P. Hennebelle, B. Godard,

F. Levrier, E. Falgarone, F. Le Petit,

E. Allys, V. Wakelam

The ISM: a multi-phase medium



(HDR P. Lesaffre)

The ISM: a multi-scale medium

- Huge dynamical range of length scales
- Equipartition between many kinds of energy

=> a multi-physics problem

	HIM	WNM	CNM	Diffuse	Dense	Discs	Sun
Density ρ [cm^{-3}]	0.004	0.6	30	200	10^4	10^{10}	1 $g.cm^{-3}$
Temperature T [K]	3.10^5	5000	100	50	10	300	10^6
Length scale L [pc]	100	50	10	3	0.1	200 AU	5.10^{-3} AU
Velocity U [$km.s^{-1}$]	10	10	10	3	0.1	0.1	1
$\mathcal{M}$	0.2	2	13	7	0.5	0.1	0.02
$\mathcal{M}_G$	130	20	15	6	0.8	0.08	0.003
$\mathcal{R}$	10^2	10^5	10^7	10^7	10^6	10^9	10^{17}
$\mathcal{R}_m$	10^{21}	10^{20}	10^{18}	10^{17}	10^{15}	10^9	10^{10}
$\mathcal{R}_{AD}$	10^3	10^3	10^2	10^3	10^4	10^5	10^{20}
Ionisation fraction	1	10^{-2}	10^{-4}	10^{-4}	10^{-4}	10^{-7}	1
Mass per ion [amu]	1	1	12	12	12	24	1
$N_e B_z$ [$3.10^{18} cm^{-2} \mu G$]	1.2	0.9	0.09	0.1	0.2	2	3×10^{16}
N_e[$10^{18} cm^{-2}$]	0.5	5	3	3	1	10^4	10^{28}

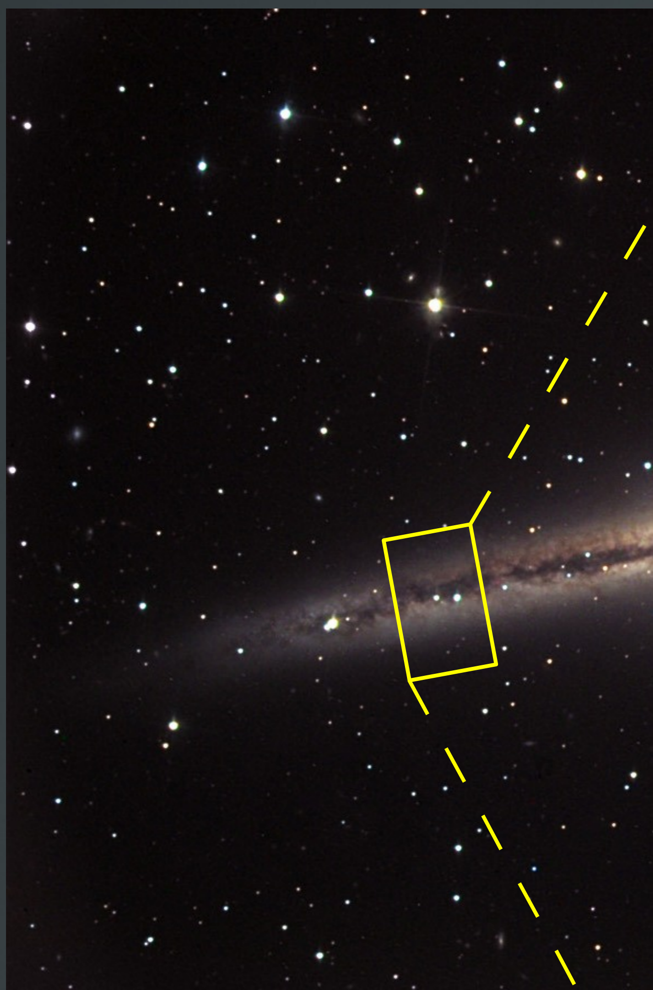
(HDR P. Lesaffre)

Global simulations of the ISM

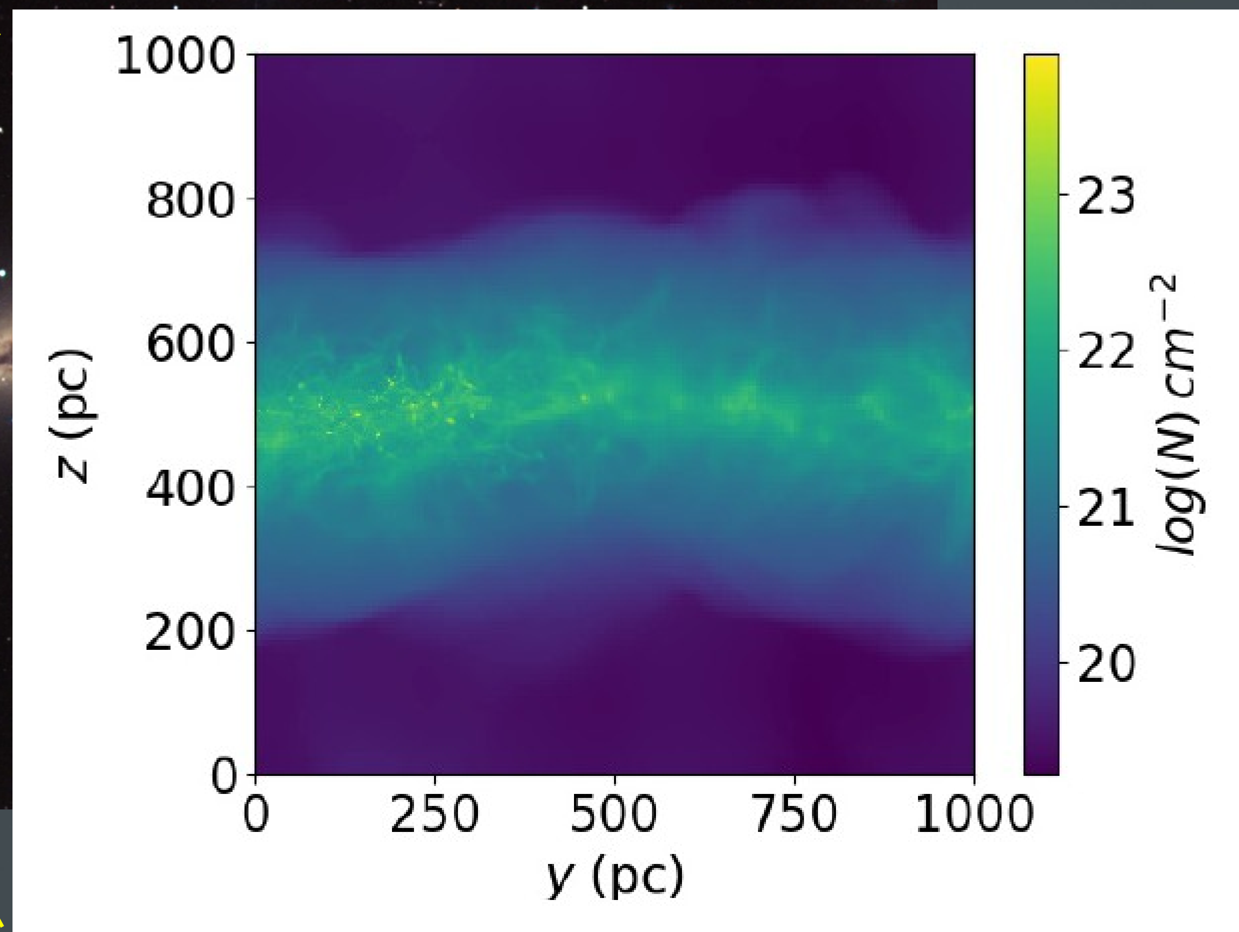
NGC 891 (AOP)

Global simulations of the ISM

RAMSES: MHD with cooling and gravity (self+galactic)



Hennebelle (2018)

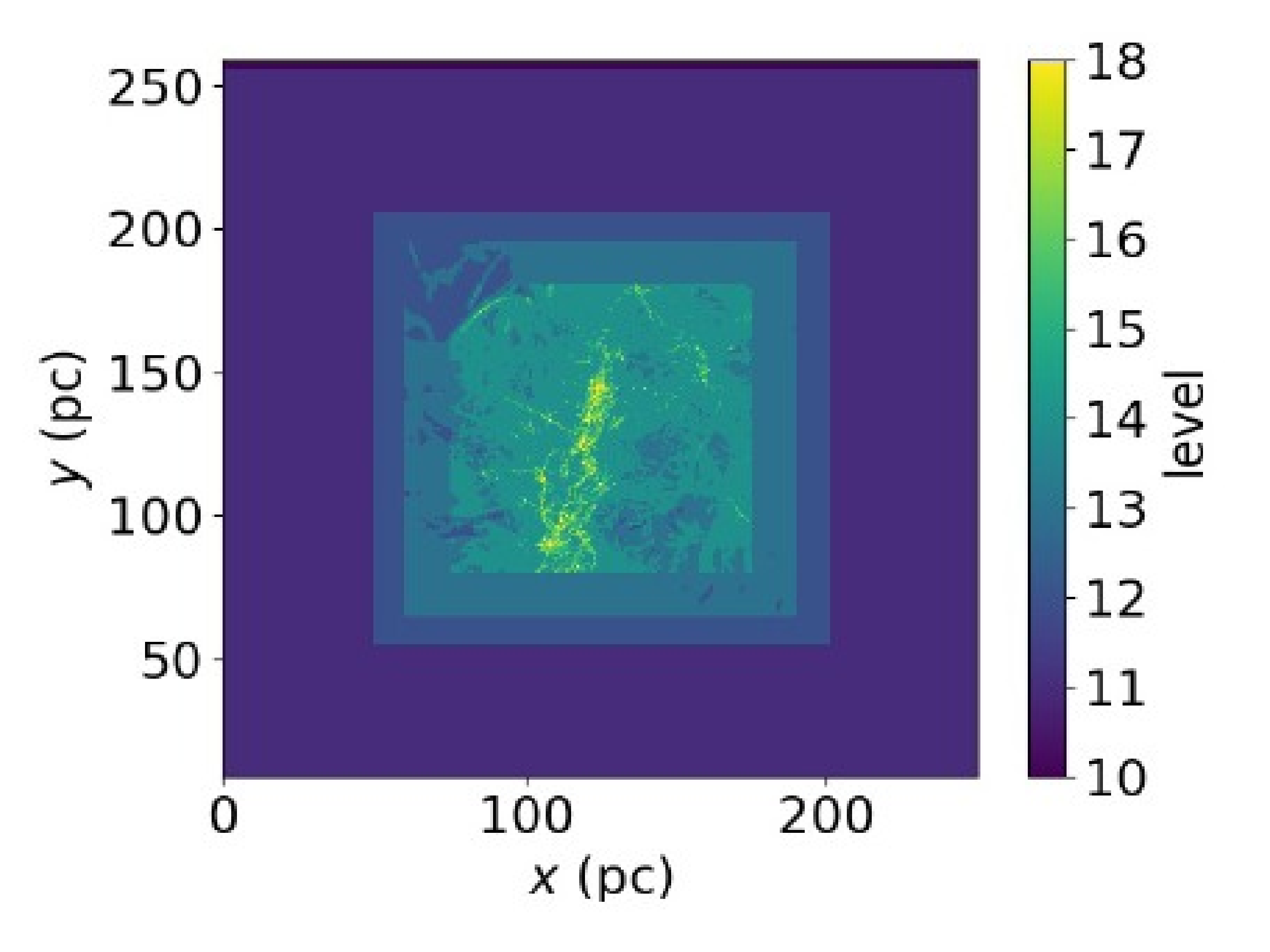


NGC 891 (AOP)

Zoom simulation

Refinement levels:
Preset zoom, plus adaptive refinement

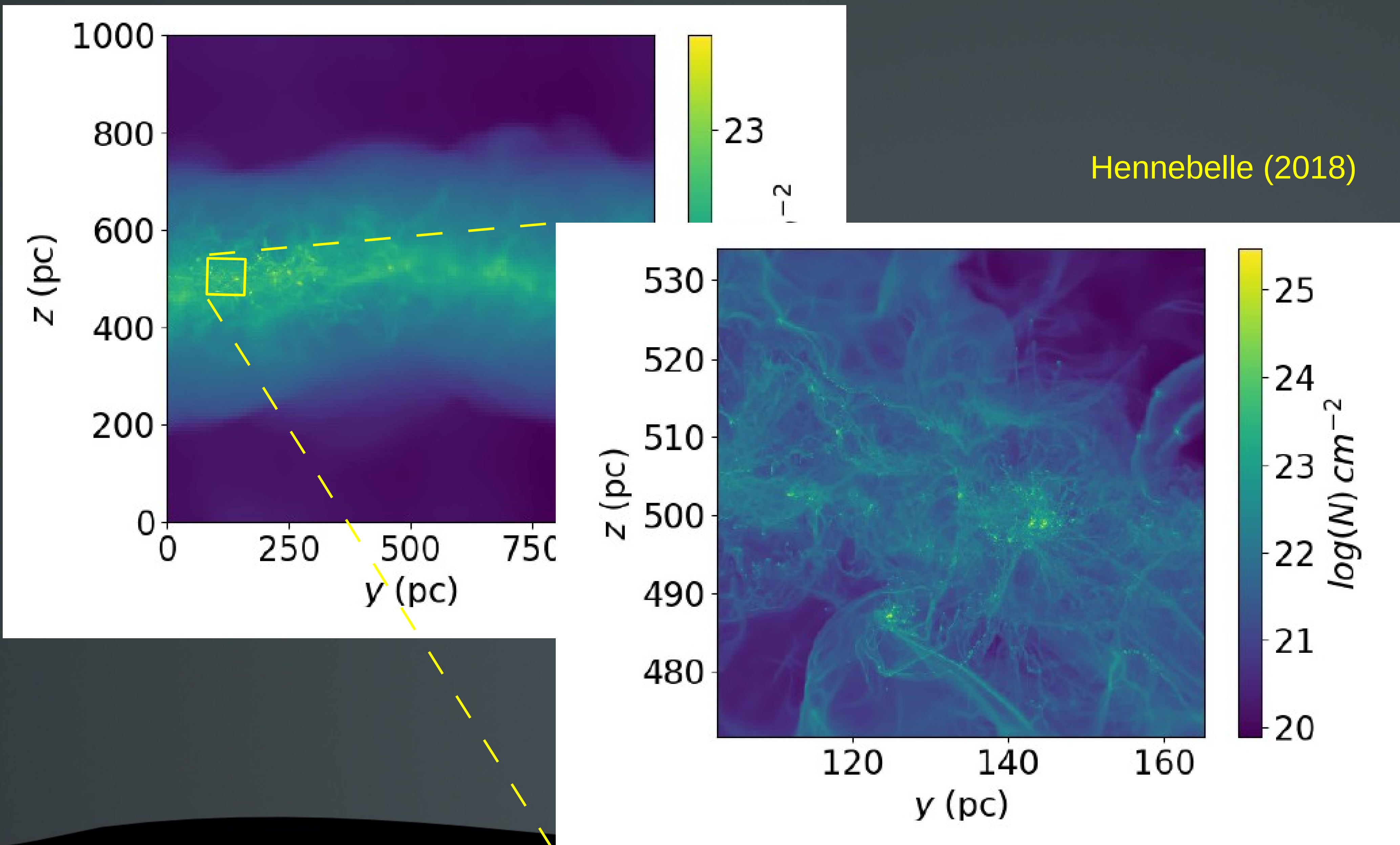
Hennebelle (2018)



Note: 18 levels
2^{18} ~ 260 000

One simulation ~ 10 Million CPU hours (PRACE project: FRIGG)

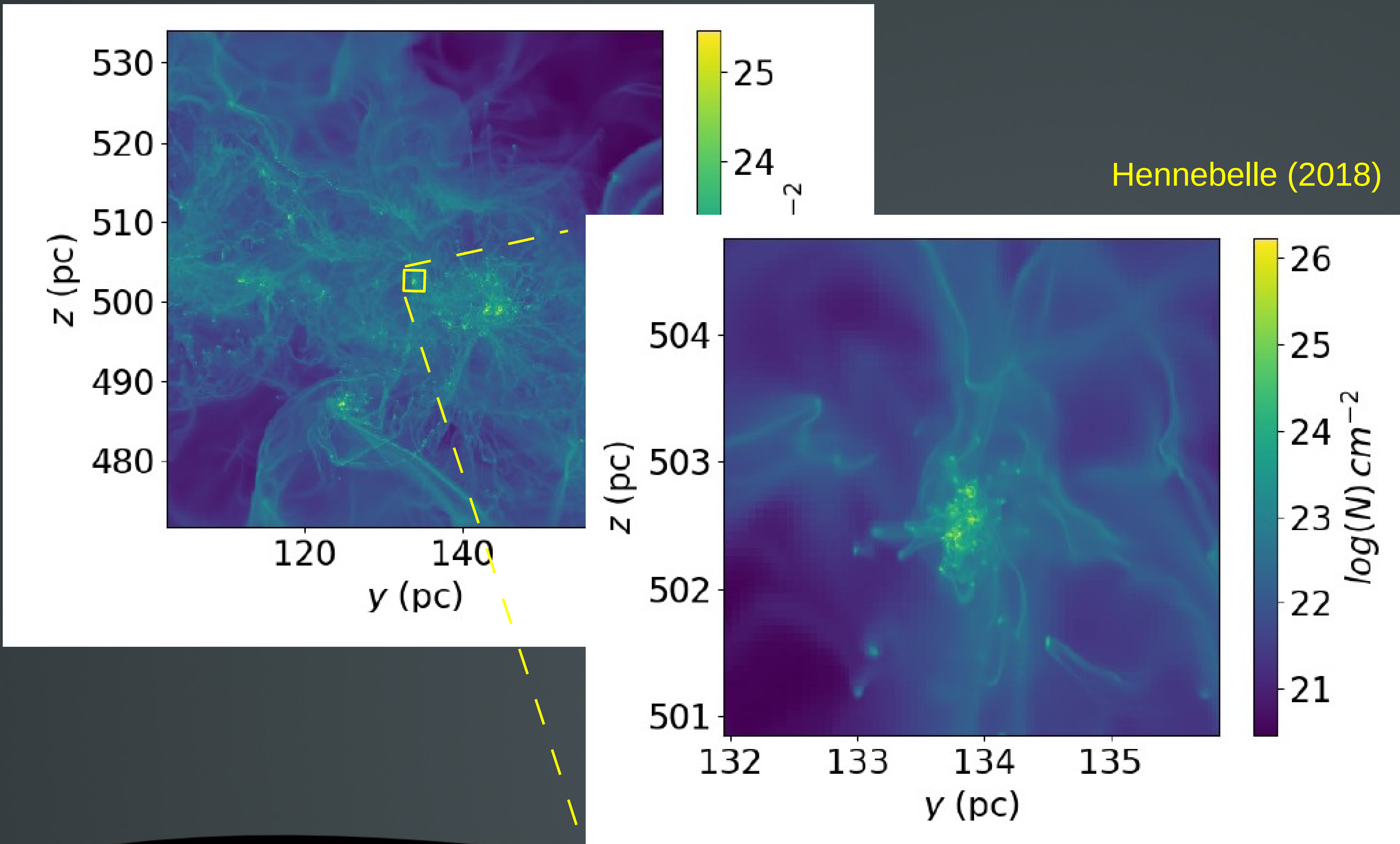
Zooming in



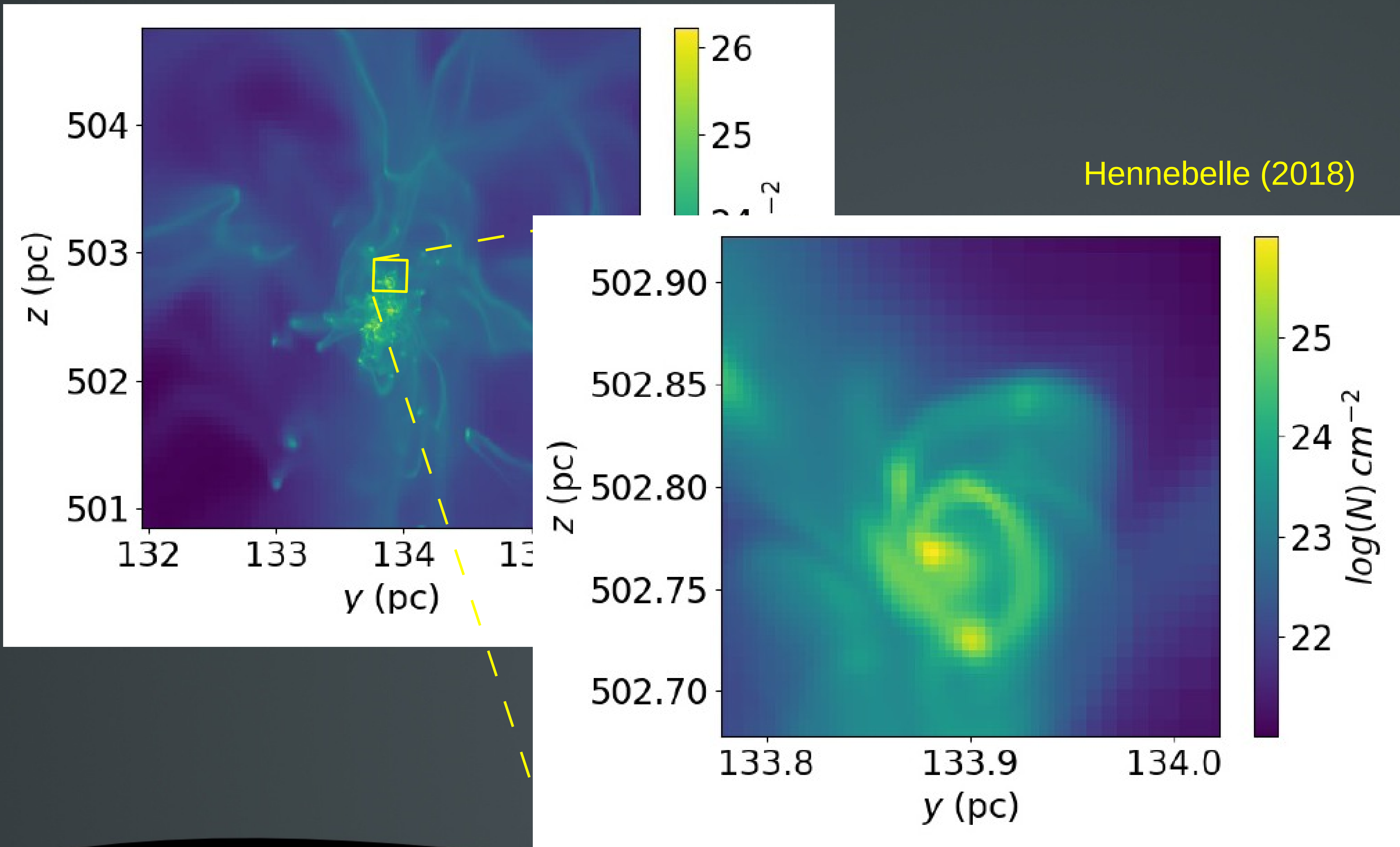
Hennebelle (2018)

Zooming in

Hennebelle (2018)



Zooming in



Hennebelle (2018)

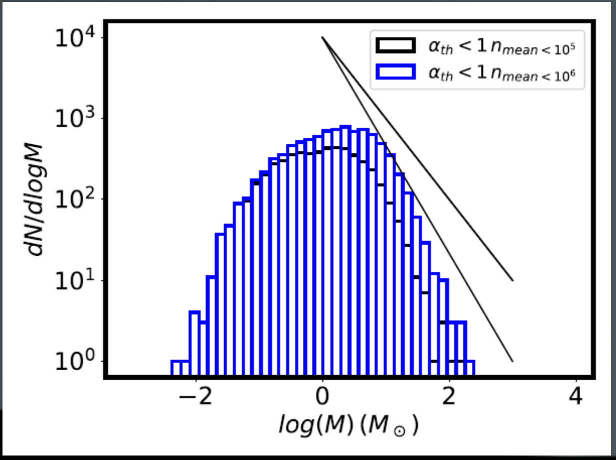
Zoom simulations

- Bridge the galactic scales and the small scales
- Provide clumps in their natural environment
- Drawbacks:

Cost, lack of numerical control (resolution effects, sticking self-gravitating pixels)

=> Huge potential for the near future

Self-gravitating
Clump statistics from
Hennebelle (2018)



Local simulations

- 100 000 CPUh each
- Homogeneous turbulence => morphology statistics
- Single objects => parameter studies
- More physics: radiative transfer (Commerçon,Valdivia), minimal chemistry (Valdivia), dissipation (Masson, Momferratos)

(Still missing: dust grains physics)

Ex: dissipation in the turbulent ISM (ERC MIST: E. Falgarone)

Origin of molecules in dilute and violent media ?

CO observed in diffuse irradiated media, Warm H_2, extragalactic (z=2) and galactic CH^+

↔ MHD turbulence dissipation ?

energy is dissipated in localised structures which may affect the chemistry and magnetic fields

=> Simulations of incompressible (pseudo-spectral) and compressible (grid-based) decaying MHD turbulence. Standard codes, focus on dissipation.

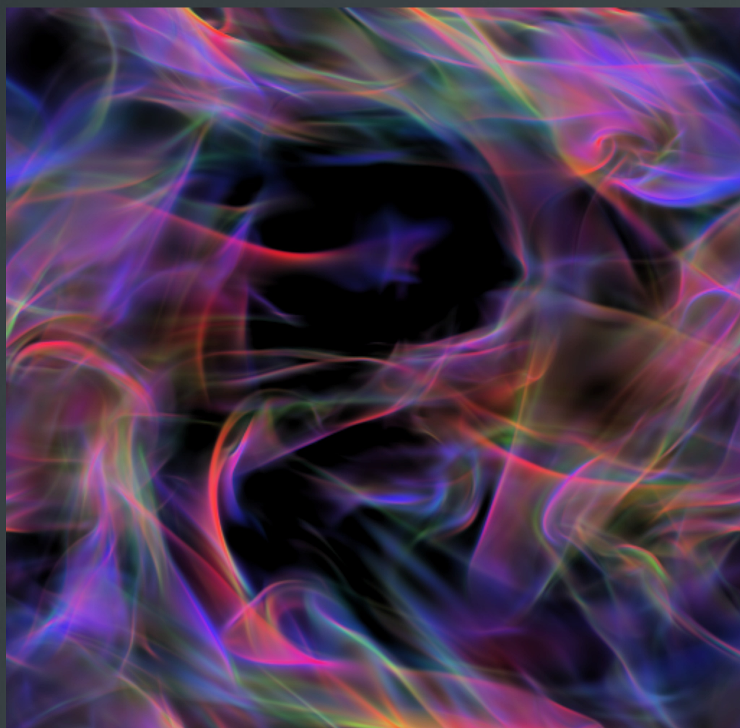
~2-3 million CPU h / yr, 640 cores ERC machine which will be incorporated in the mesoPSL pool.

Ex: dissipation is dominated by incompressible modes

Projection of dissipative heating in the plane of sky around time of peak total dissipation

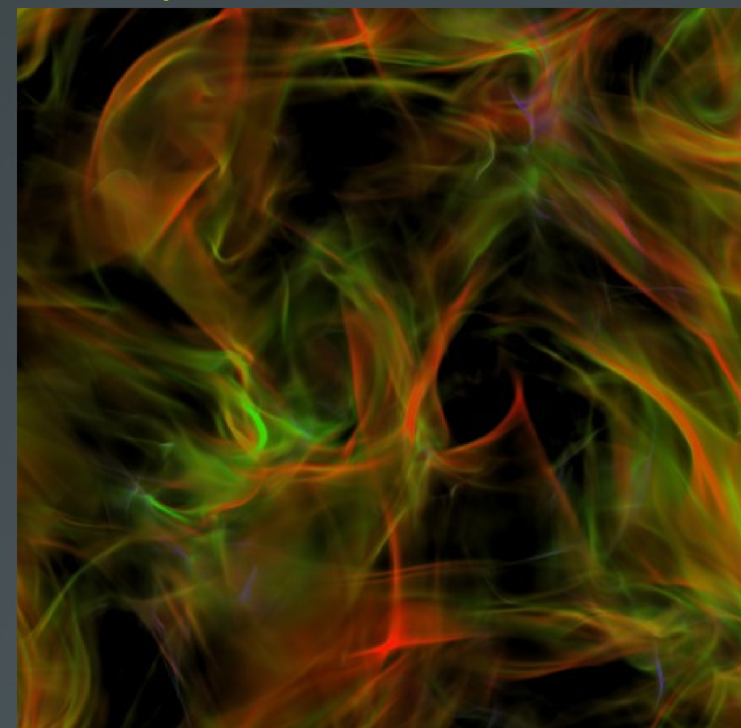
Mach 0

1 pc



Ohmic, Viscous, Ambipolar

Mach 4



Ohmic, Viscous incompressible
Viscous compressible

- Dissipation happens on sheets which project as ridges on the sky
- Structures are similar in compressible and incompressible runs
- Most dissipation happens at small convergence (-div(u) small)

Link to observations: which data representation ?

Van Gogh: la nuit étoilée

Link to observations: which data representation ?

- Bitmap
- Fourier spectrum
- Clump/filaments statistics
- Intermittency signatures
- Wavelet scattering coefficients
- Reduced wavelet scattering coefficients (Allys+2019)

Data statistical reconstruction

(Allys+2019, *submitted*)

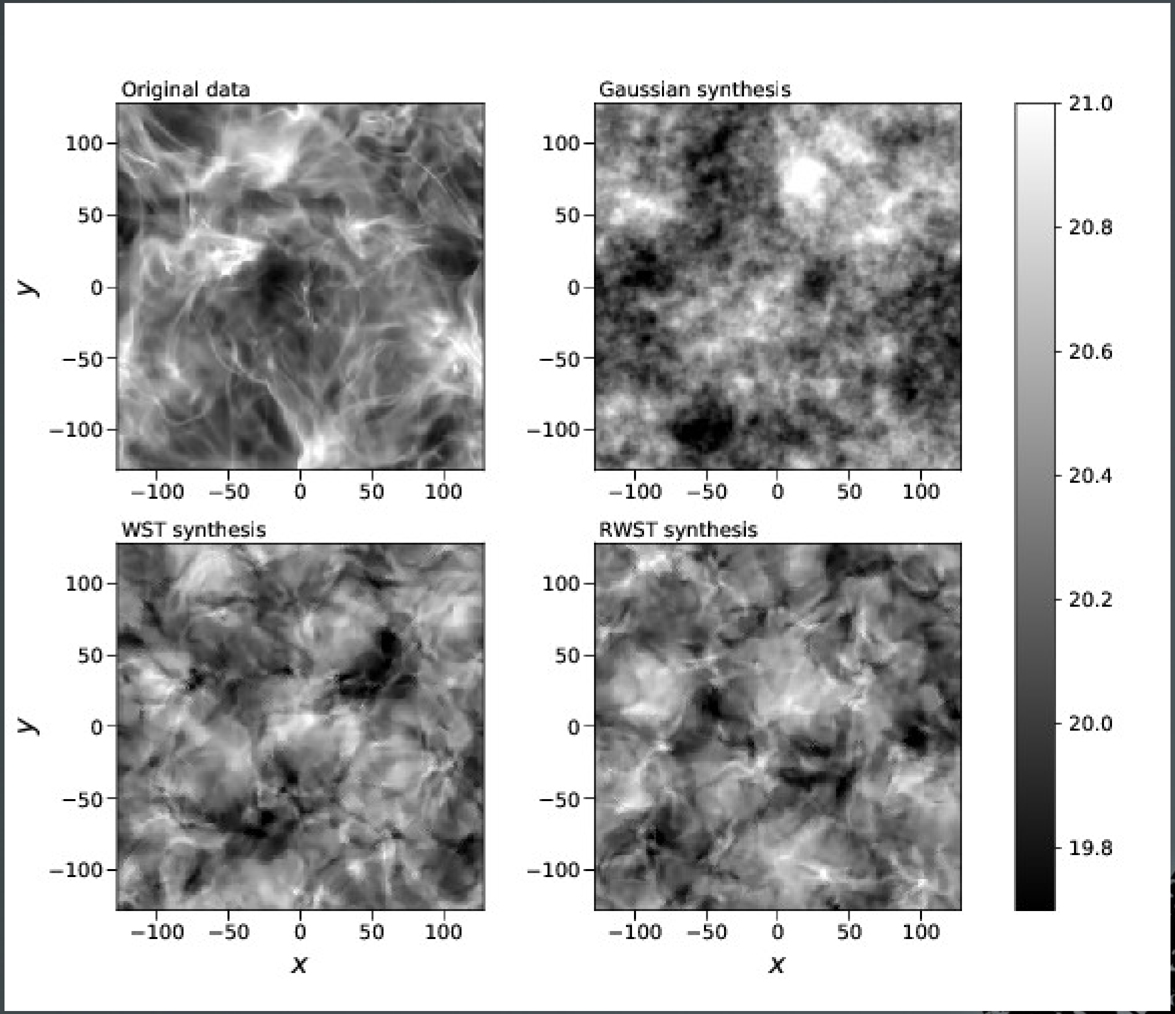
(1 out of 20 projections of snapshots of a MHD simulation)

Same power spectrum
Random phases

(10^6 coeffs)

(50 coeffs)

(N.B.:
All images have same mean and variance)



(1000 coeffs)

(70 coeffs)

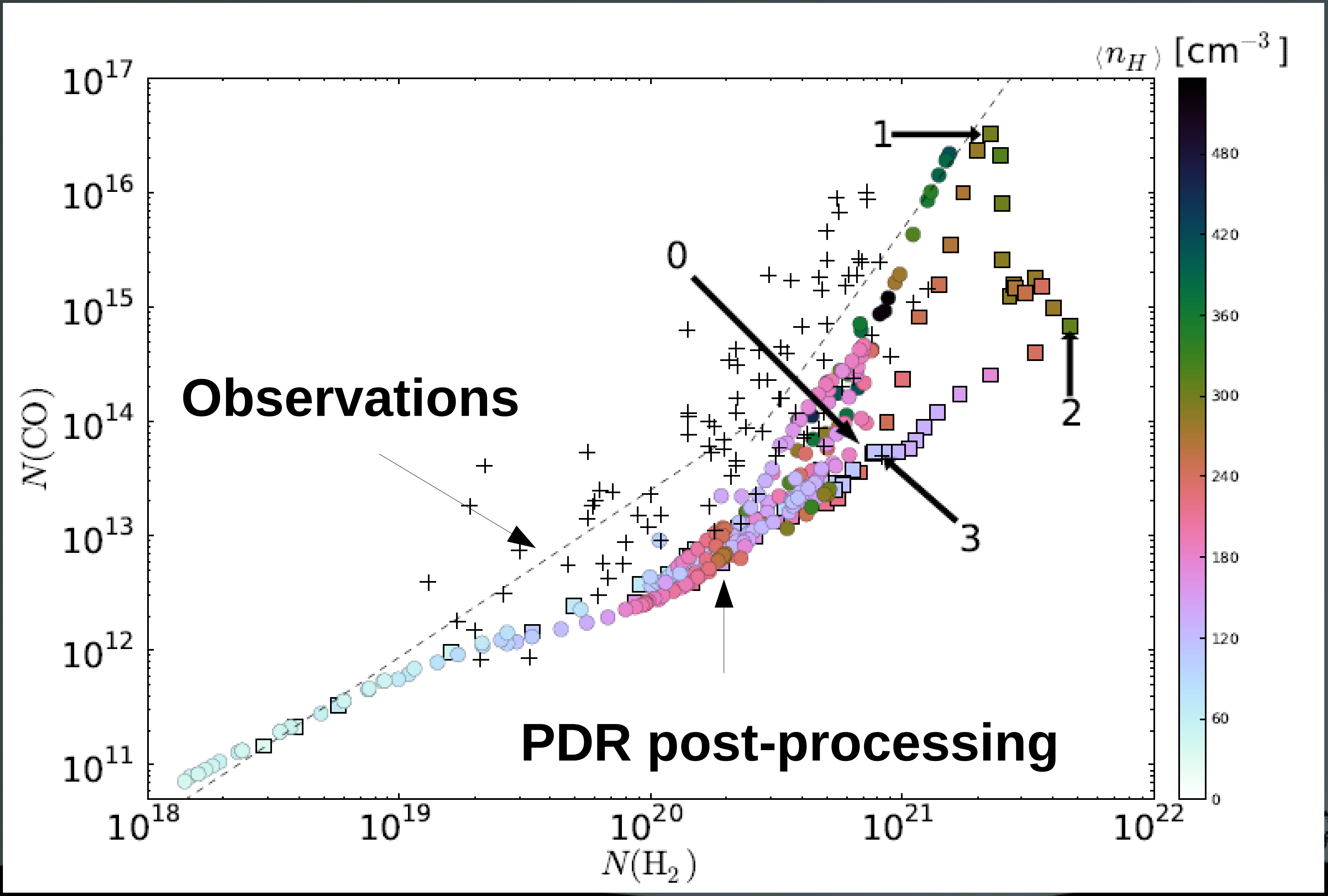
Same Wavelet
Scattering Coefficients

Same Reduced Wavelet
Scattering Coefficients

1D ↔ 3D Painting the simulations

ex: Levrier+2012, PDR post-processing

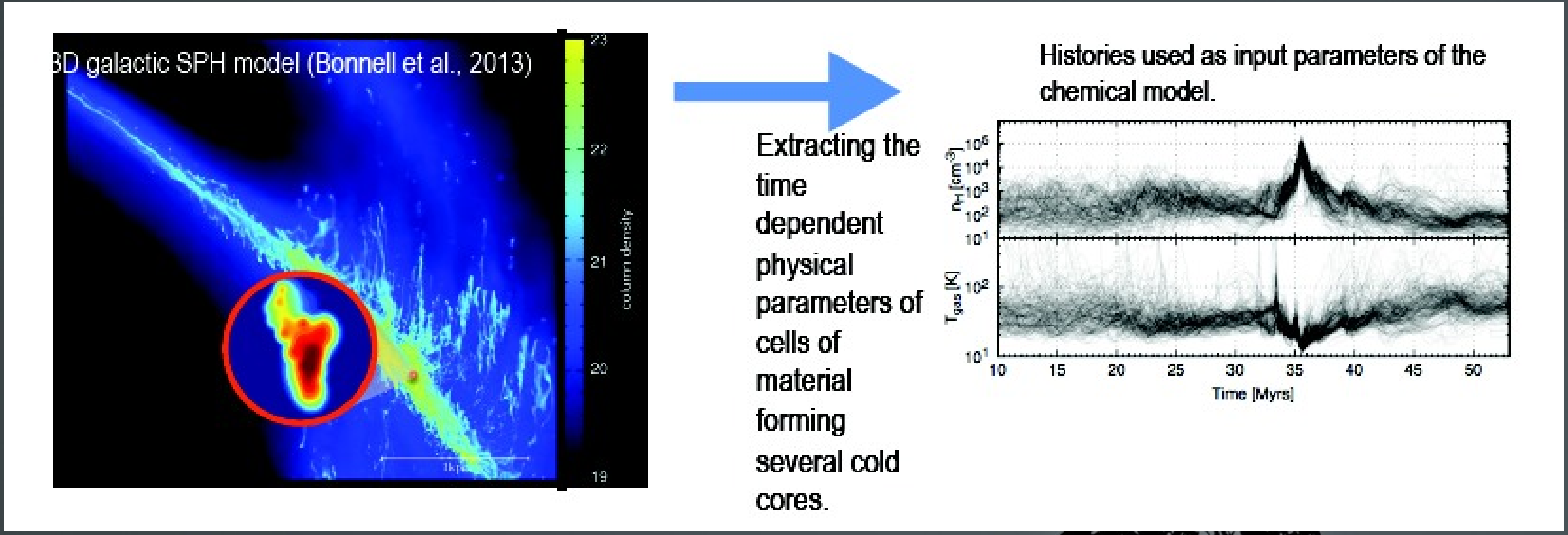
Multiphase simulations ρ(l.o.s.) ↔ 1D Meudon PDR code



1D ↔ 3D Painting the simulations: going closer to the observations

- *Eulerian*: detect steady structures (e.g. shocks) and model them (0D/1D)
- *Lagrangian*: replay (T,ρ) history of fluid parcels (0D)

Ex: Ruaud+2018

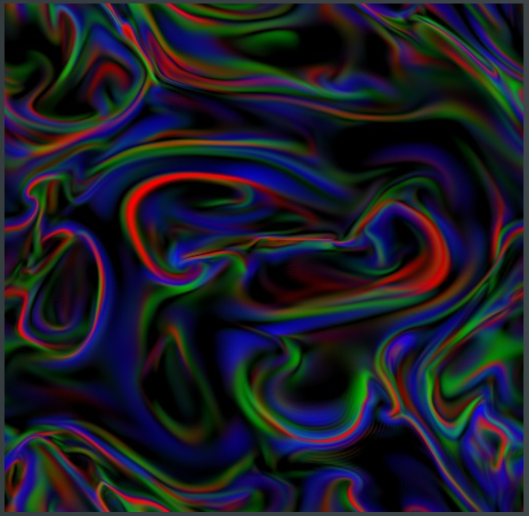


Credits: V. Wakelam

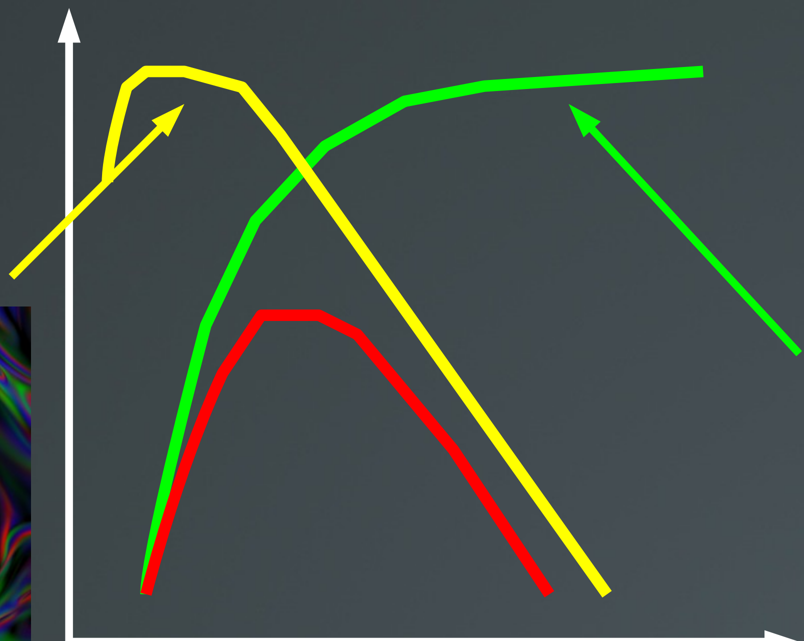
=> Efforts to design Sub-grid models

1D ↔ 3D Prospects

Intermittent statistics of the dissipation

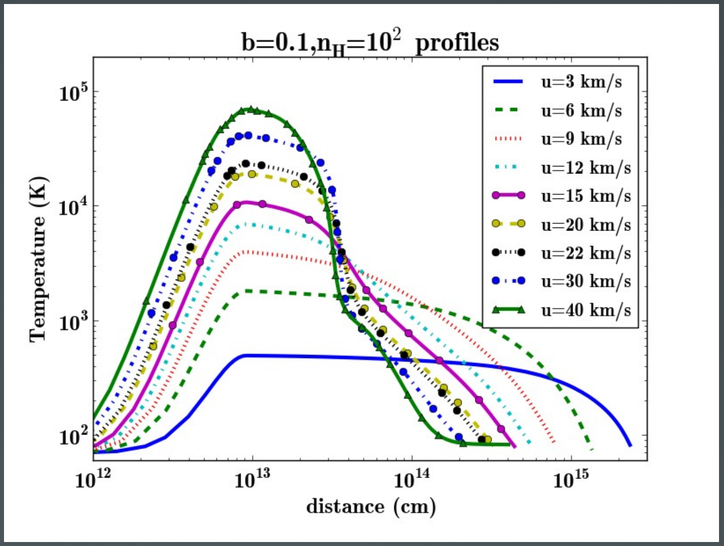


3D simulations
(cf Momferratos et al. 2013)

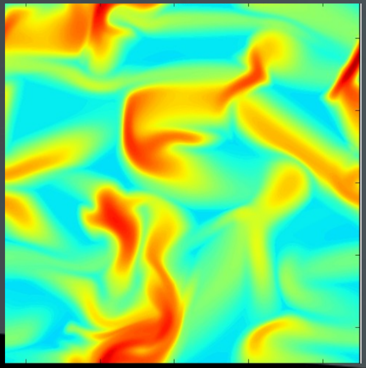


=> Molecules
Formation + excitation

Molecular yields from Shocks (for example)



1D simulations



CO map

<u>*Validation with 2D simulations*</u>

1D/0D models

- Few minutes CPU on a laptop => huge grids
- Can incorporate detailed microphysics
- Complex radiative transfer
- Detailed chemistry (gas, grain, state-to-state)
- Bin size by bin size dust growth / fragmentation / adsorption / desorption / sputtering / erosion
- Need advances in the underlying microphysics

PDR Code
The Meudon PDR code

DustEM
Dust Emission

Shock
Paris-Durham Shock model

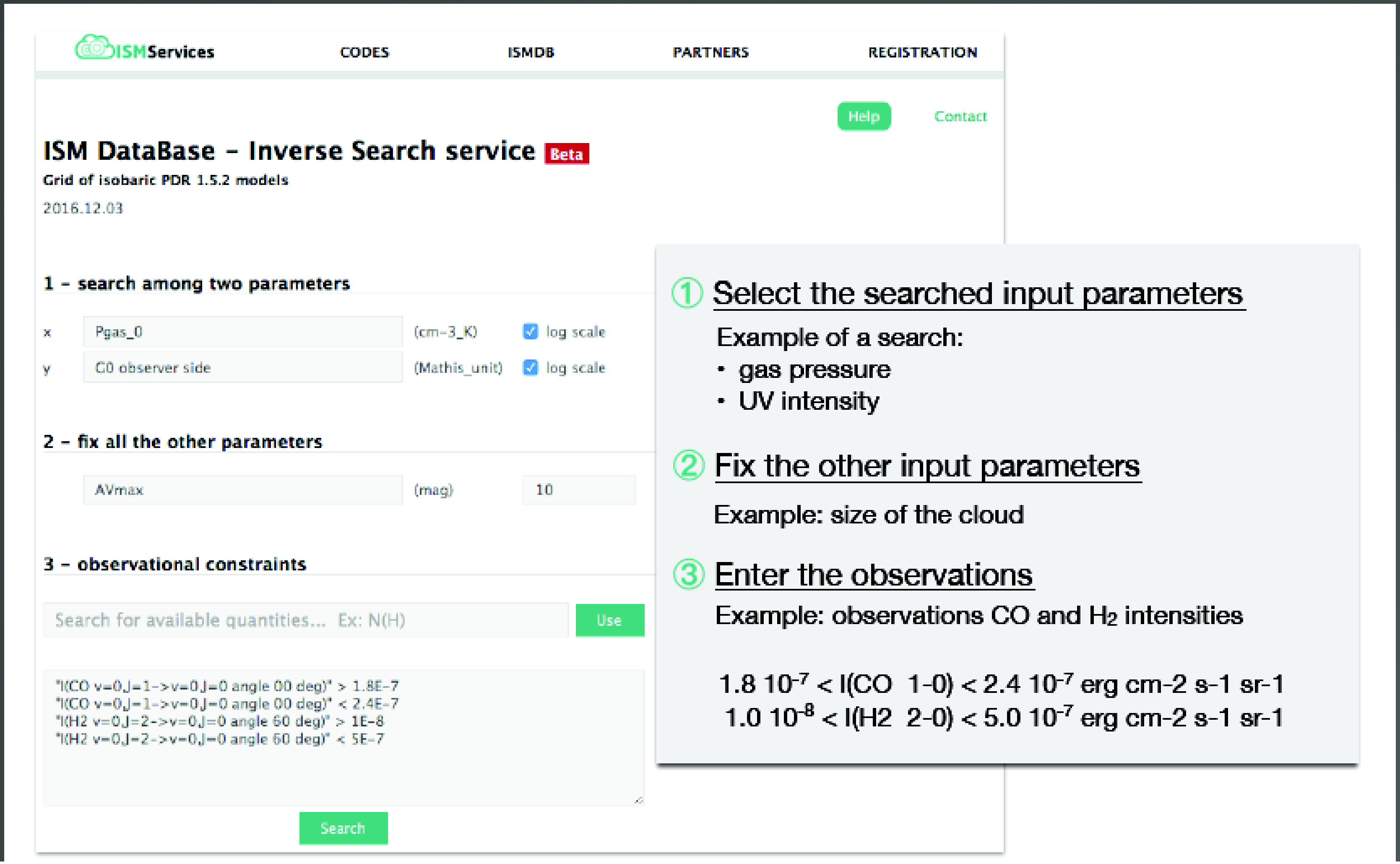
Starformat
MHD simulations data base

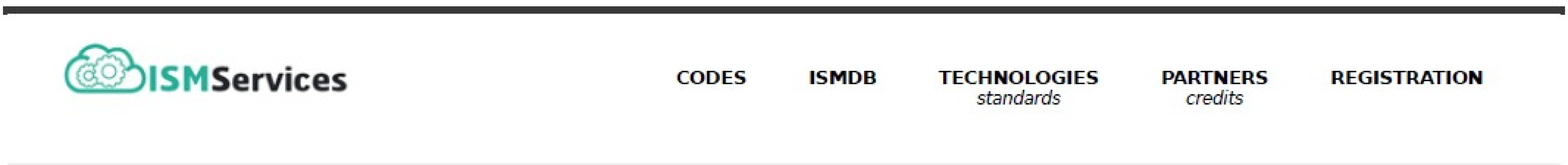
http://ism.obspm.fr

http://ism.obspm.fr

ISMDB

Credits: F. Le Petit





Collisional Rates computation

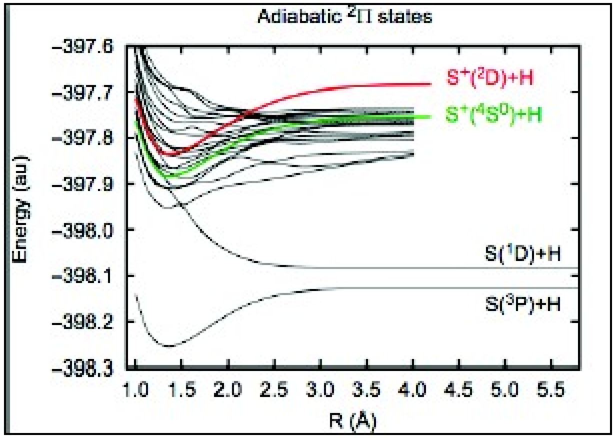
Large range of computational needs:

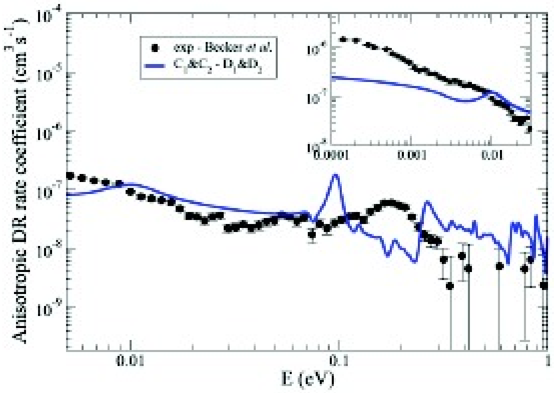
$10^3 - 10^7$ CPU hours

- Potential energy surface
  - *Ab initi*o methods
  - Gold standard: CCSD(T)
  - Commercial codes (e.g. MOLPRO)
  - Parallel
  - N^7 scaling (N the system size)
  - Sampling ~ 10 000 geometries
  - 1 geometry is 1-10 CPU hour
  - Memory < 100 GB
- Scattering dynamics
  - Quantum treatment
  - Gold standard: close-coupling
  - Public codes (e.g. MOLSCAT)
  - Parallel
  - N^3 scaling
  - Sampling: 100-1000 energies
  - 1 energy is 10-100 partial waves
  - 1 partial wave is 1-100 CPU hour
  - Memory > 1 TB for large systems

Credits: A. Faure

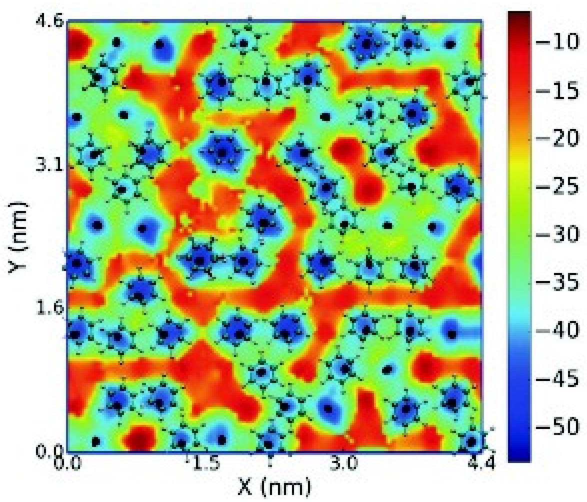
Ex: recent advances in theory vs. XP comparisons





Gas phase astrochemistry

Excellent agreement between calculated and experimental SH^{+} + e- dissociative recombination rate coefficients D. *Kashinski et al. JCP 2017*



Solide state astrochemistry

Map of adsorption sites for benzene on an ISM ice. *E. Michoulier et al. PCCP 2018*

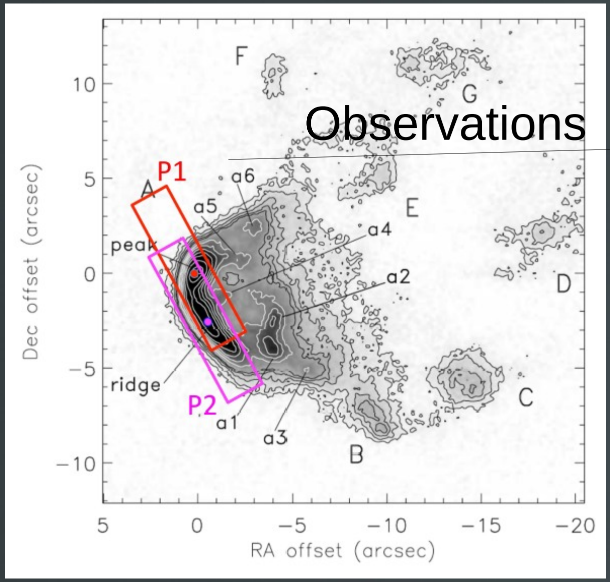
Credits: A. Faure

Dust Physics: everywhere through the galactic cycle

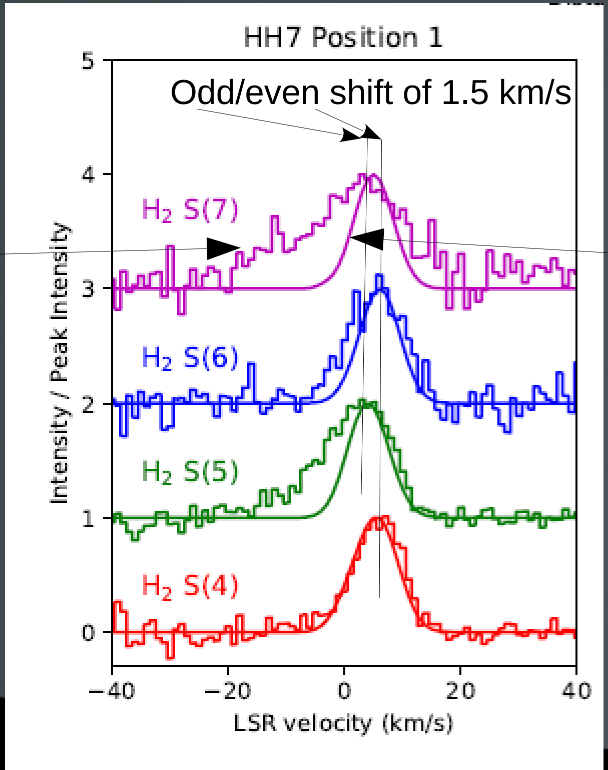
- Controls radiated energy during star formation
- Catalyst for H_2
- Ices & path to molecular complexity=> grain surface chemistry
- AGB winds launching => feedback
- Coupling to B field: ionisation degree, mass loading
- Planck foregrounds, polarisation & B structure
- Dust spinning and disruption (see recent Thiem + Tram 2018-2019 papers)

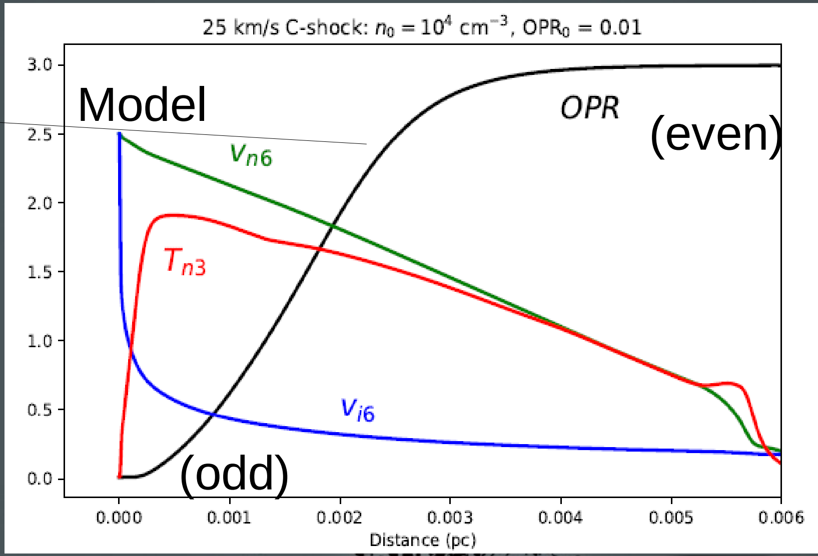
Line shapes probe chemical and dynamical information

- Line shifts explained by H_2 ortho/para rise in decelerating gas (Neufeld+19, *submitted*)
- Broadening by thermal Doppler and velocity range
  =>Future: 3D modeling as in Tram+2018



HH7 EXES observations





Paris-Durham shock model

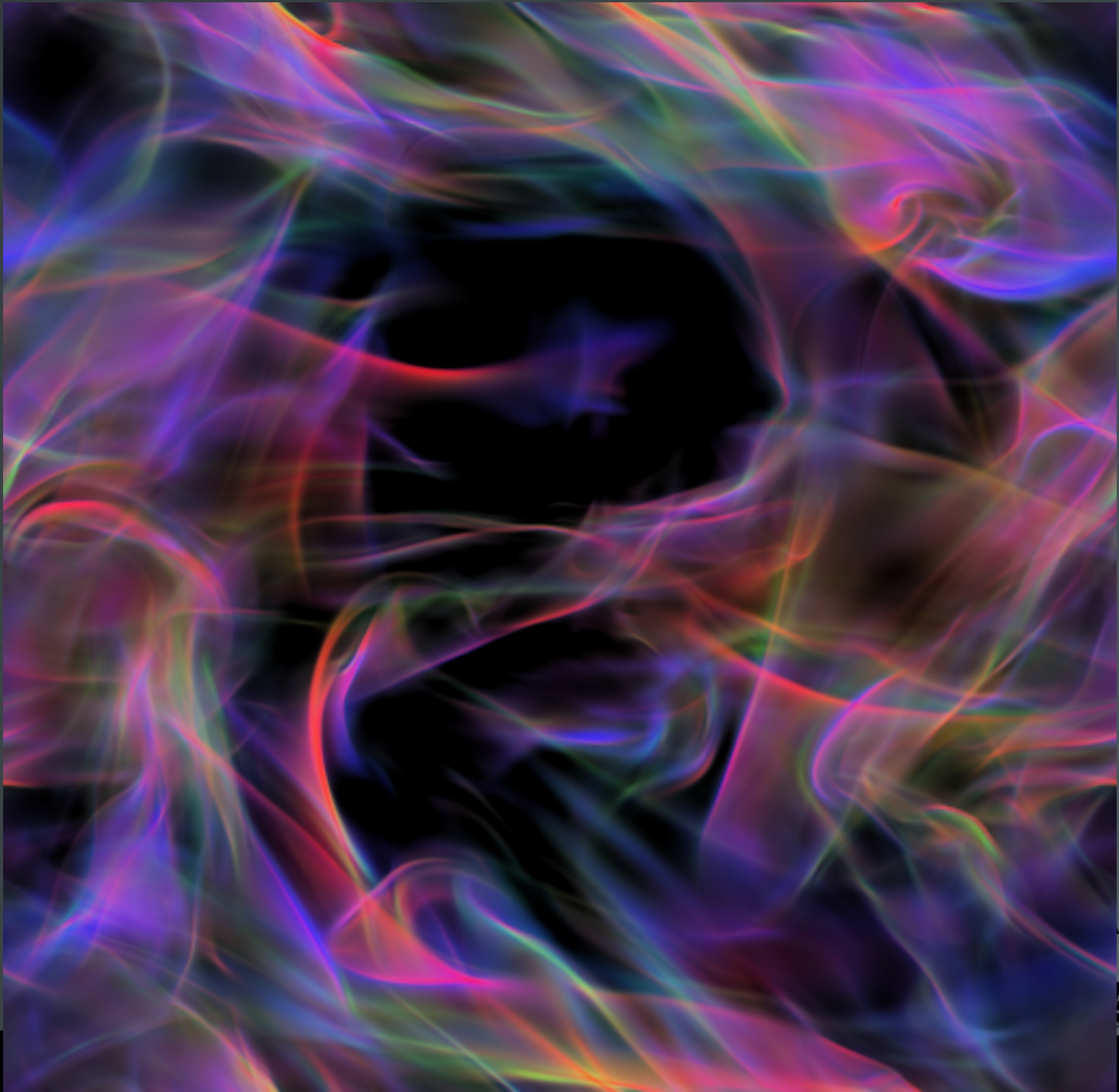
Exascale challenge

- New hardwares (ARM vs x86 architectures) motivated by smartphones and video games
- Towards more cores with less power spent
- Hybrid mixture of cores

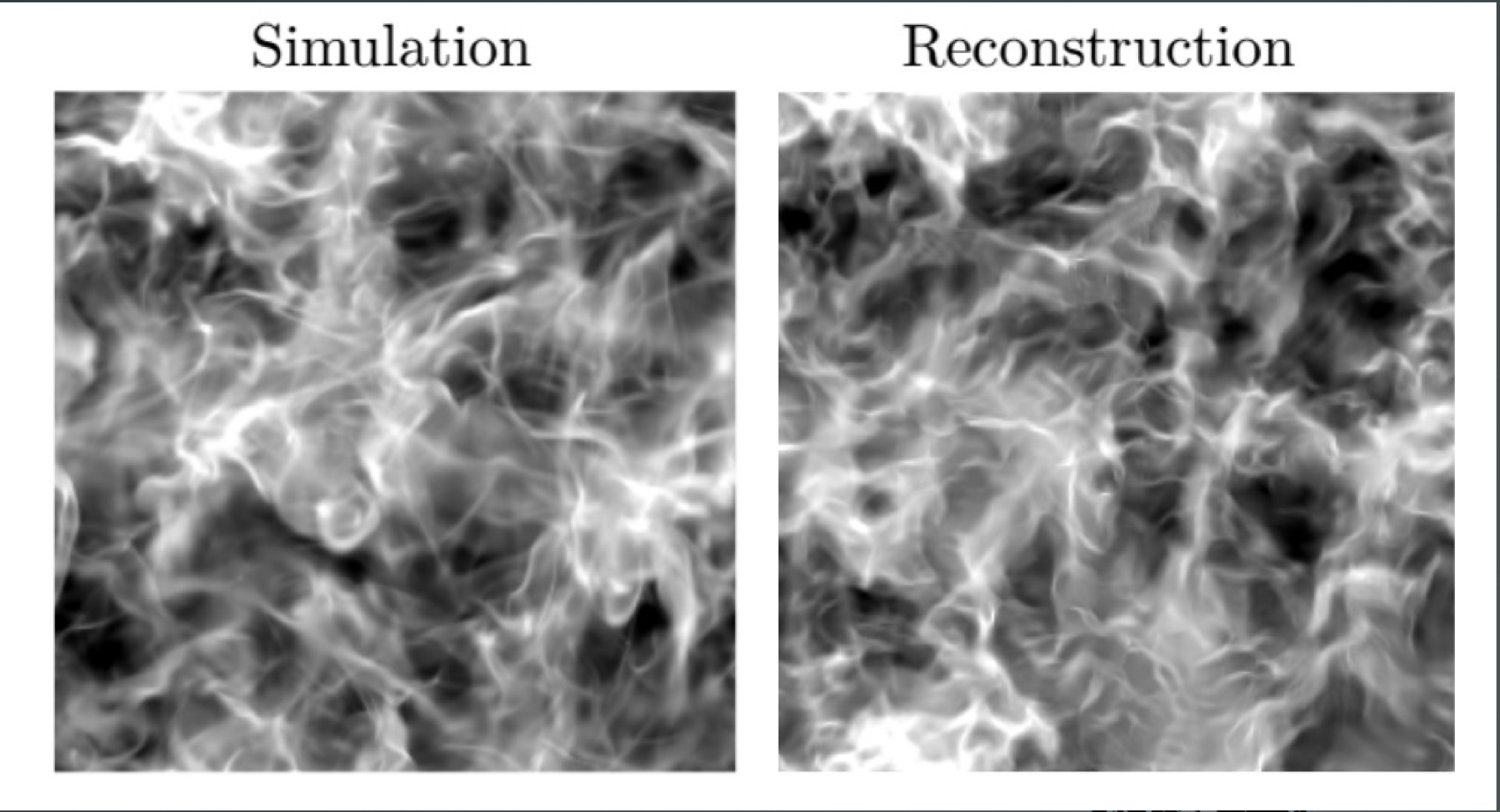
=> We need good engineers and to talk to them

(ex: DUMSES for GPU by M. Joos)

THANKS !



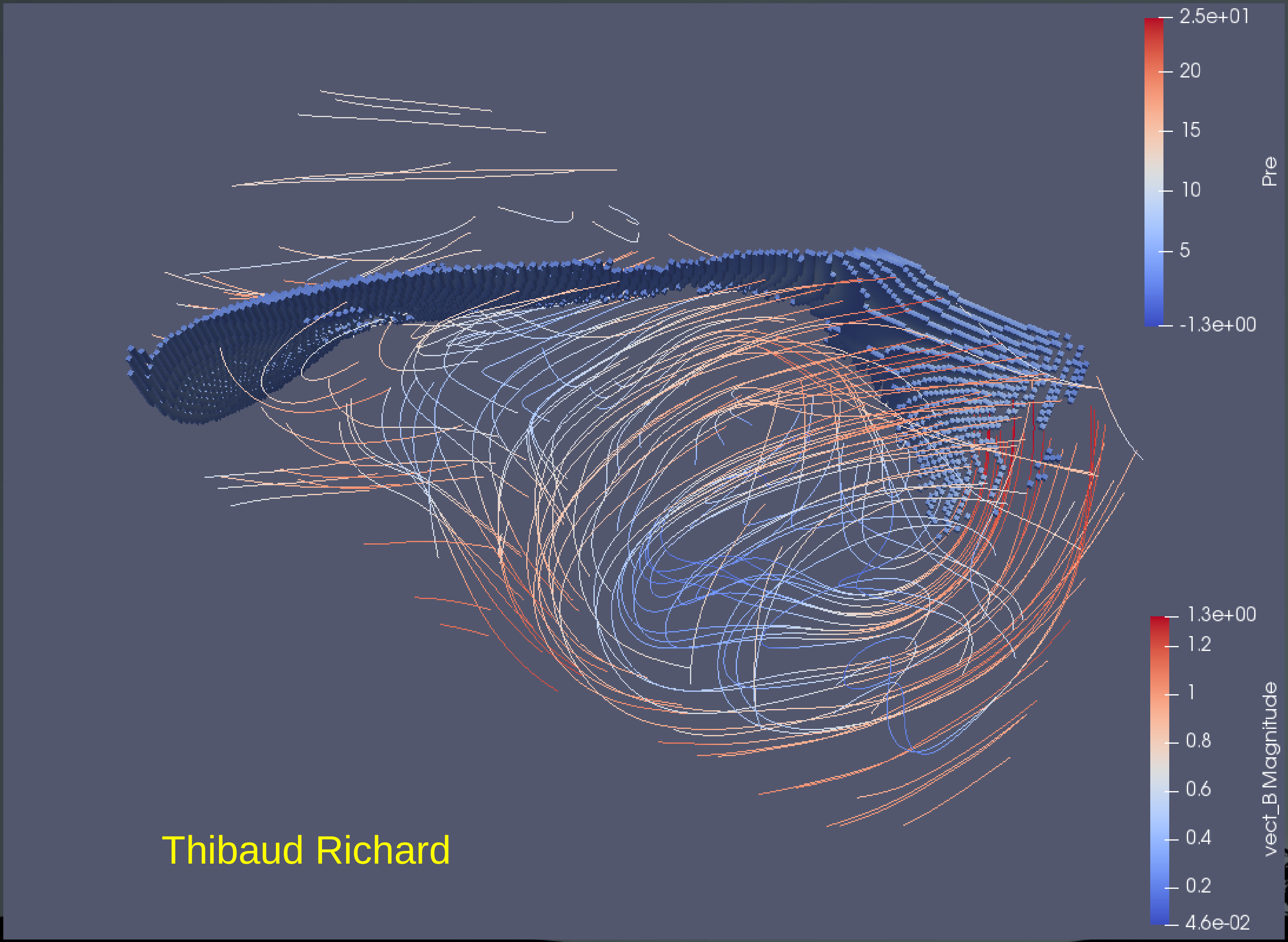
Harmonic phases synthesis (S. Mallat)



And it needs only one image...

Dissipative structures extraction

Find connected sets where dissipation > mean + n.std



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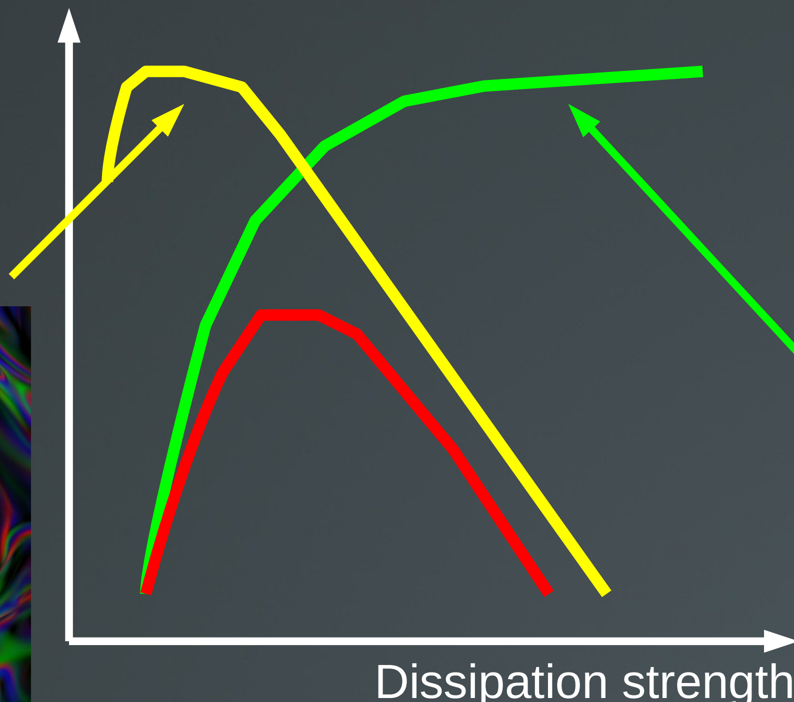
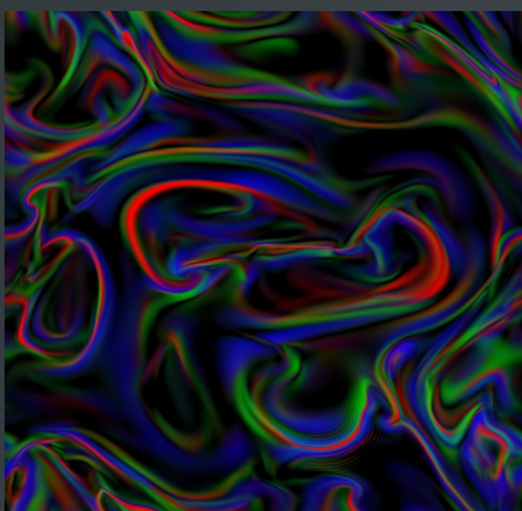
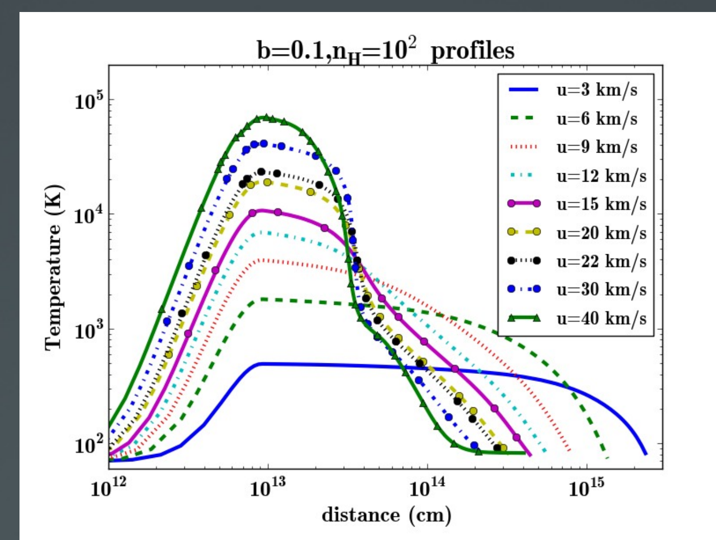


Molecular yields from Shocks (for example)

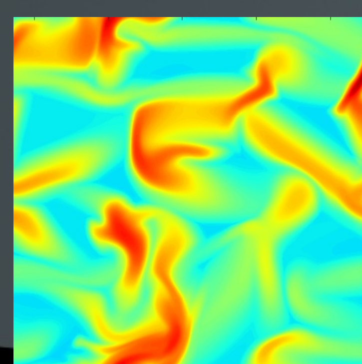


3D simulations
(cf Momferratos et al. 2013)

=> Molecules Formation + excitation



1D simulations



CO map

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