(Some) Modeling tools for the ISM

The Eagle Nebula (NASA, ESA, and The Hubble Heritage Team STScI/AURA)

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IYAS « Large ground-based 21th century radio instruments: ALMA/NOEMA/SKA/LOFAR/NenuFAR » - 17/11/2015

The Cycle of interstellar matter

Stars

$n > 10^{22}\ \mathrm{cm}^{-3}$

Stellar winds, Planetary Nebulæ, Supernova remnants, ...

NGC2440 with HST
(K. Noll / STScI)

Crab Nebula with HST
(A. Loll et al. / STScI)

Heavy Elements
Kinetic energy

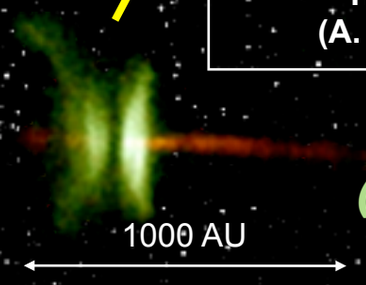
Cosmic rays

Large scale energy injection

Radiation

Hot ionized gas (HIM)

$n \sim 10^{-2}\ \mathrm{cm}^{-3}, T \sim 10^{6}\ \mathrm{K}$



HH30 with HST
(A. Watson / STScI)

Protostellar objects (accretion disks, jets...)

1000 AU

Warm ionized gas (WIM)

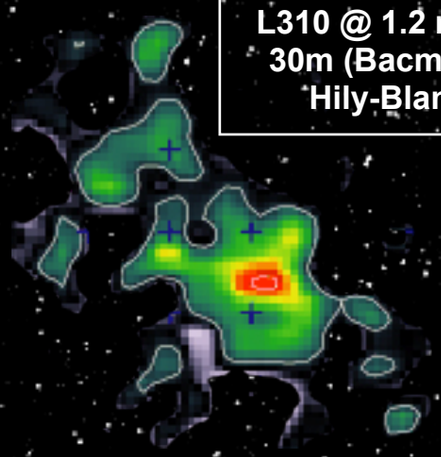
$n \sim 0.5\ \mathrm{cm}^{-3}, T \sim 8000\ \mathrm{K}$

Molecular gas

$n \sim 10^{3}\ \mathrm{cm}^{-3}, T \sim 10\ \mathrm{K}$

Warm neutral gas (WNM)

$n \sim 0.5\ \mathrm{cm}^{-3}, T \sim 8000\ \mathrm{K}$

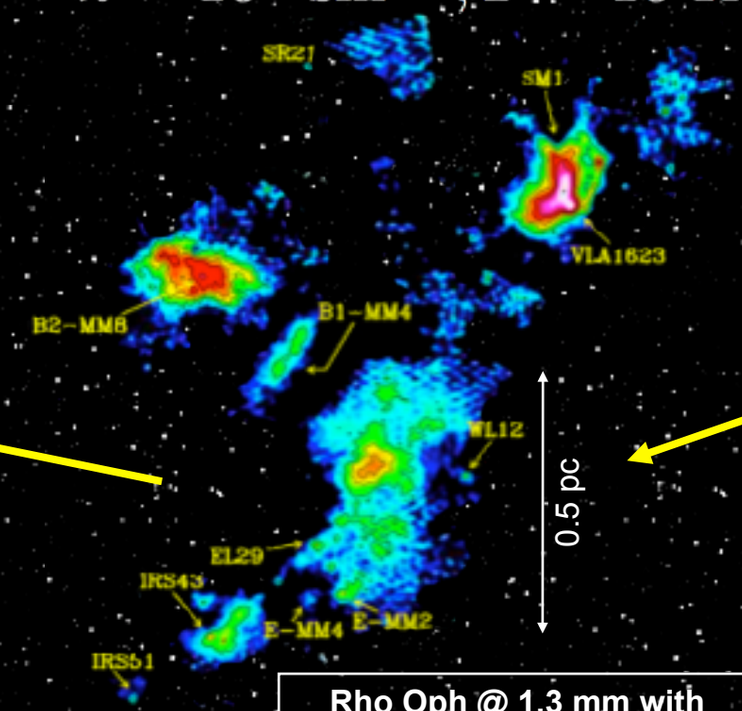


L310 @ 1.2 mm with IRAM
30m (Bacmann et al. '00,
Hily-Blant et al. '10)

0.05 pc

Dense cores

$n \sim 10^{6}\ \mathrm{cm}^{-3}, T \sim 10\ \mathrm{K}$



Rho Oph @ 1.3 mm with
IRAM 30m (Motte et al. '98)

Cold neutral gas (CNM)

$n \sim 10^{2}\ \mathrm{cm}^{-3}, T \sim 10^{2}\ \mathrm{K}$

... and dust grains

MHD, microphysics, gravity, turbulence, thermodynamics, chemistry, particle physics...

The ISM : an open and complex system

A variety of processes, with comparable strengths…

- **Self-gravity** See S. Bontemps' talk
- **Turbulent dynamics** See F. Bournaud's talk
- **Magnetic fields** See F. Boulanger's talk
- **Radiation**
- **Chemistry** See M. Gerin's talk

… over large dynamic ranges

- **Density fluctuations**
- **Spatial and temporal scales**
- **Coupling of scales and processes**

OUT OF THIS WORLD

A wealth of molecules is found in interstellar clouds

2 atoms		3 atoms		4 atoms		5 atoms	
H_2	NO	C_3	MgCN	c-C_3H	HNCS	C_5	HC_2NC
AlF	NS	C_2H	MgNC	l-C_3H	HOCO$^+$	C_4H	HCOOH
AlCl	NaCl	C_2O	N_2H^+	C_3N	H_2CO	C_4Si	H_2CHN
C_2	OH	C_2S	N_2O	C_3O	H_2CN	l-C_3H_2	H_2C_2O
CH	PN	CH_2	NaCN	C_3S	H_2CS	c-C_3H_2	H_2NCN
CH$^+$	SO	HCN	OCS	C_2H_2	H_3O^+	CH_2CN	HNC_3
CN	SO$^+$	HCO	SO_2	HCCN	NH_3	CH_4	SiH_4
CO	SiN	HCO$^+$	c-SiC_2	HCNH$^+$	SiC_3	HC_3N	H_2COH^+
CO$^+$	SiO	HCS$^+$	CO_2	HNCO			
CP	SiS	HOC$^+$	NH_2				
CSi	CS	H_2O	H_3^+				
HCl	HF	H_2S	SiCN				
KCl	SH	HNC	AlNC				
NH	FeO	HNO					

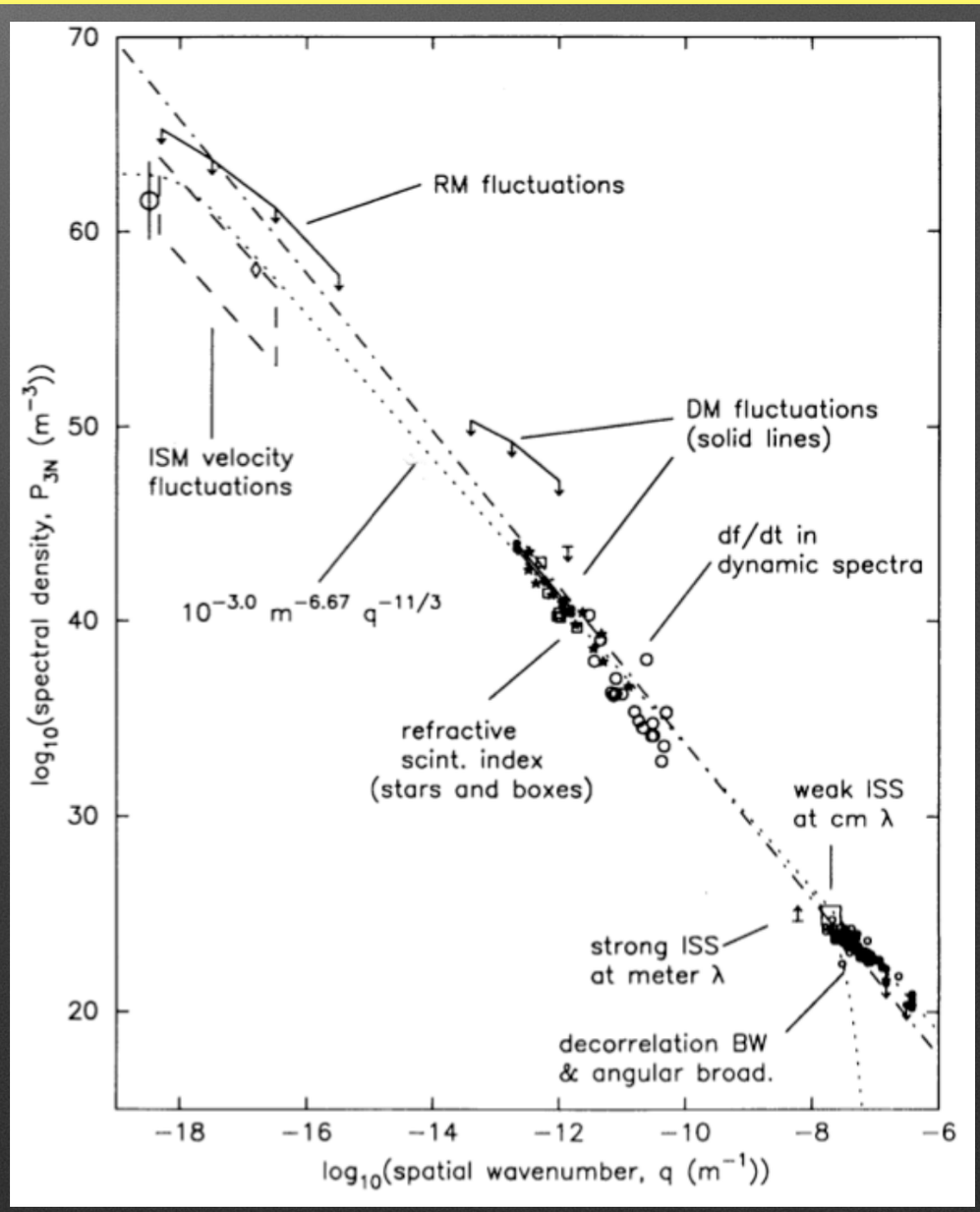
6 atoms		7 atoms	8 atoms	9 atoms
C_5H	CH_3SH	C_6H	CH_3C_3N	CH_3C_4H
l-H_2C_4	HC_3NH^+	CH_2CHCN	HCOOCH$_3$	CH_3CH_2CN
C_2H_4	HC_2CHO	CH_3C_2H	CH_3COOH	$(CH_3)_2O$
CH_3CN	NH_2CHO	HC_5N	C_7H	CH_3CH_2OH
CH_3NC	C_5N	HCOCH$_3$	CH_2OHCHO	HC_2N
CH_3OH		NH_2CH_3		C_8H
		c-C_2H_4O		
		CH_2CHOH		

10 atoms	11 atoms	13 atoms
CH_3C_5N	HC_9N	$HC_{11}N$
$(CH_3)_2CO$		
NH_2CH_2COOH		

NOTE: Evidence suggests that much larger molecules such as polycyclic aromatic hydrocarbons and fullerenes are also present.
SOURCE: National Radio Astronomy Observatory

About 200 species detected in the ISM

Electron density in local ISM (Armstrong et al., 1995)



A galaxy of modeling codes, modules, and packages

Chemistry

KROME
Nahoon
Nautilus

PDR

Cloudy_3D
Cloudy
Leiden
UCL
3D-PDR
Meudon

Gas dynamics

ENZO
FLASH
HERACLES
GADGET-2
Hyperion
ZEUS
AREPO
Athena
GIZMO
RAMSES
CHOLLA
PLUTO
AZeus
EMMA
Dedalus

Hybrid / Specific

Fervent
CHEMSES
MOCASSIN
KM2
TPCI
Torus-3D
MODA
RAMSES-RT
Paris-Durham

Radiative transfer

RADEX
DustEM
RADMC
LIME
DustPol
Hyperion
RH-1.5D
SHAPEMOL
STOKES
SALT

Aspects of ISM modeling

Gas dynamics

- Grid-based (e.g. RAMSES) or particle-based (e.g. GADGET)
- With or without self-gravity
- Mono- or multi-fluid

Radiative transfer

- Monte-Carlo methods (e.g. RADMC)
- Moment methods (e.g. RAMSES-RT)
- Large velocity gradient (LVG) methods (e.g. RADEX)

Chemistry

- Steady-state (e.g. Meudon PDR) or time-dependent (e.g. Nahoon)
- Gas-phase only (e.g. Nahoon) or including grain surface processes (e.g. Nautilus)

Instrumental effects

- Bandpass filtering
- Spatial filtering

Challenge is in the coupling

Gas dynamical simulations

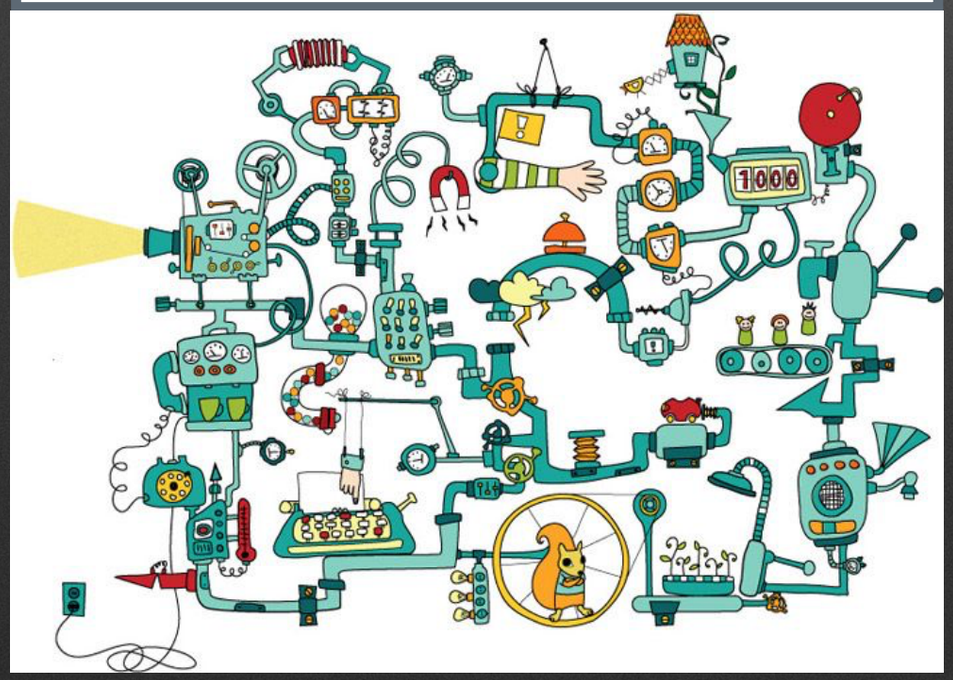
- Large range of spatial scales, requiring large 3D grids
- Time-dependent evolution of gas density, velocity, magnetic field, …

Micro-physical and chemical models

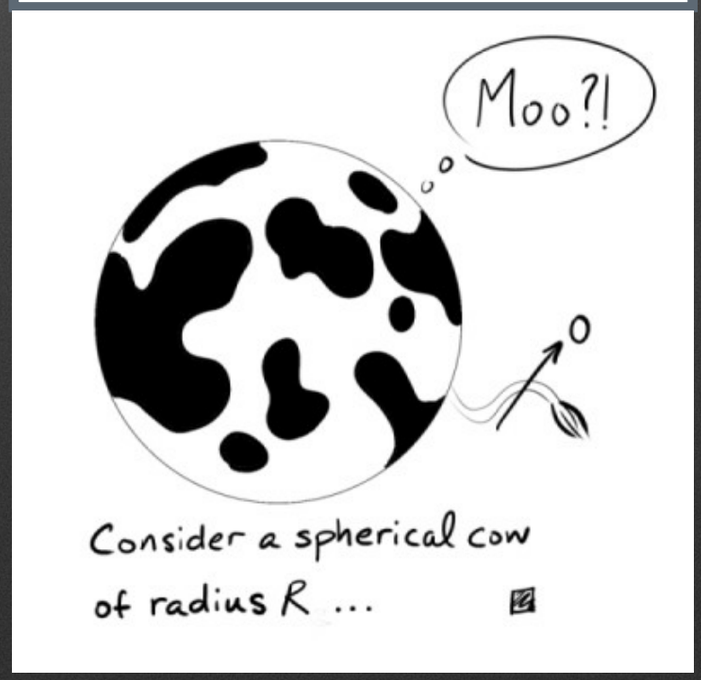
- Many chemical species and reactions
- Thousands of energy levels and corresponding lines
- Light-matter interactions

A detailed gas-dynamical and microphysical simulation is beyond our reach

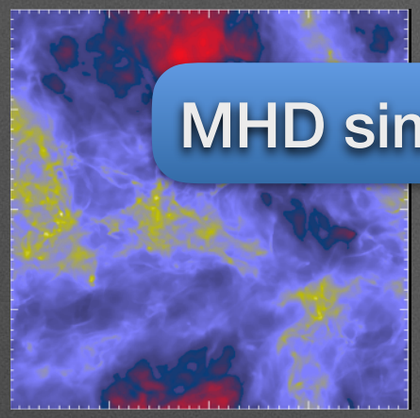
Post-processing of gas-dynamical simulations



Coupling of simplified codes



A workflow view of ISM modeling



MHD simulation

Density profiles

Meudon PDR
chemical structure

UV spectrum

Abundances,…

Radiative transfer

DustEM
grain physics

Dust properties

Line intensites

Instrument simulator

VAMDC
Atomic and molecular physics database

The Interstellar Medium Platform

ISMServices

http://ism.obspm.fr

- **Meudon PDR** code and database
- **DustEM** dust emission models
- **Paris-Durham** shock code
- **STARFORMAT** MHD simulation database

- State-of-the-art numerical codes
- Databases of pre-computed models
- Analysis tools

l'Observatoire de Paris Virtual Observatory Paris Data Centre

irap astrophysique & planétologie

CRA Lyon

ASTRONET www.astronet-eu.org

pcmi physique et chimie du milieu interstellaire

DE LA RECHERCHE À L'INDUSTRIE cea

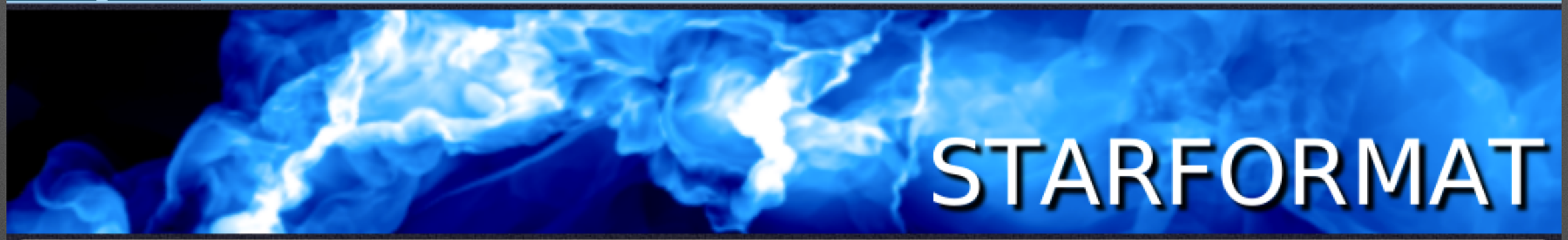
IAS Institut d'Astrophysique Spatiale Orsay

GSO DATA CENTRE OBSERVATOIRE VIRTUEL GRAND SUD OUEST

ZAH

The STARFORMAT database

SIMULATIONS | DESCRIPTION



The StarFormat DataBase

The StarFormat database contains results of heavy numerical simulations computed in order to study the problem of star formation, essentially molecular cloud formation, evolution and collapse.

Understanding the dynamical evolution of the interstellar medium (ISM) and its relation to stellar birth is a key challenge in astronomy and astrophysics. The **STAR FORMAT** project aims at providing observers and theorists studying formation and evolution of molecular clouds, their morphological and kinematical characteristics, and the formation of stars in their interior with a set of theoretical tools and a database of models to aid in the analysis and interpretation of current and future observations.

The goal of this database is to give access to observers, or more generally to any scientist working on a related field, to the results of these numerical simulations, which could be useful to help prepare or analyze observations.

Available projects:

PROJECT	DESCRIPTION
Molecular cloud evolution with decaying turbulence	This project aims at describing the evolution of a turbulent molecular cloud in which the turbulence is decaying.
Barotropic dense core simulations	This project aims at describing the gravitational collapse of magnetized molecular dense cores.
Colliding flow simulations	This project aims at describing self-consistently the formation of molecular clouds starting from the very diffuse atomic interstellar medium.
Solenoidal vs. Compressive Turbulence Forcing	This project investigates the influence of different forcing (i.e., kinetic energy injection) on turbulent flows in the interstellar medium.

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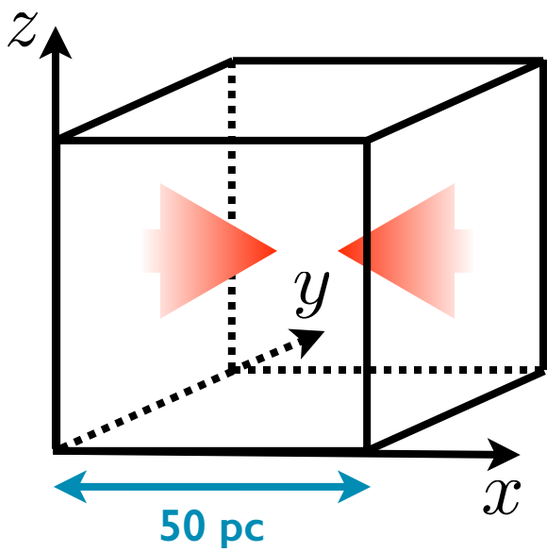
OPEN DATA

http://starformat.obspm.fr

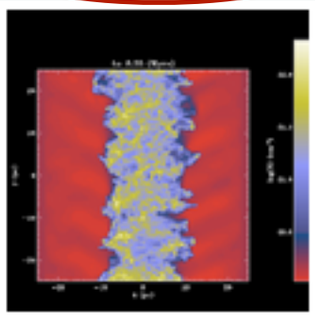
Example data extraction from STARFORMAT



Head-on collision of two warm neutral gas flows at supersonic speeds

t = 8.55 MYRS

Column density along the z axis



EXTRACT AND DOWNLOAD SNAPSHOT DATA

Snapshot statistics for cells above a threshold in density or column density

STATISTICS ON ALL CELLS WITH Density ≥ 0

Mean Magnetic Intensity	7.12 microGauss
Mean Density	6.17 cm^{-3}
Total Mass	2.622×10^4 solar mass
Mean Pressure	1.837×10^{-12} $erg.cm^{-3}$
Mean Temperature	1.704×10^3 K

What kind of values do you want to extract?

- a projection of column density
- a slice of density
- a slice of pressure
- a slice of velocity
- a slice of magnetic field

along which axis?

- X
- Y
- Z

Extraction size: 50,000 pc

(50,00 pc for the whole simulation, the number of cells along each axis is 2)

Centered on: X 25,000 (pc) Y 25,000 (pc) Z 25,000 (pc)

Precision L_{max}: 10 corresponding to a resolution of 0.048 pc/cell

(maximum L_{max} allowed for this size of extraction: 10)

E-mail address (to receive a link to download the results):

Results fileformat: ASCII BIN FITS HDF5

Extract Reset Cancel

PROPERTY PLOTS

- Column Density in XY
- Column Density in XZ
- Column Density in YZ
- Density cut in XY
- Density cut in XZ
- Density cut in YZ
- Magnetic Intensity in XY
- Magnetic Intensity in XZ
- Magnetic Intensity in YZ
- Magnetic Intensity Variance vs. Density
- Magnetic Intensity vs. Density
- Mass vs. Column Density
- Mass vs. Density
- Pressure cut in XY
- Temperature cut in XY
- Temperature Variance vs. Density
- Temperature vs. Density

Download ASCII data

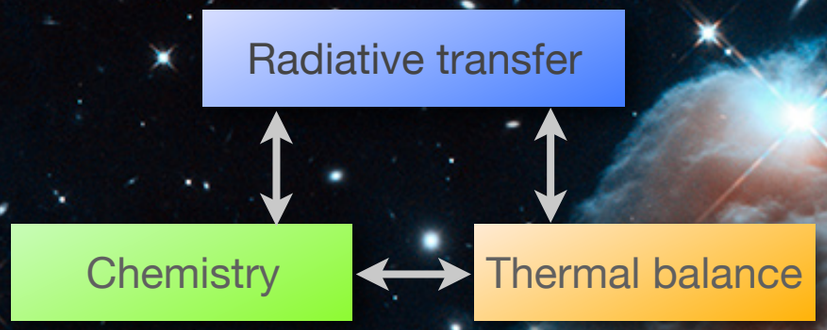
Download PNG plot or image

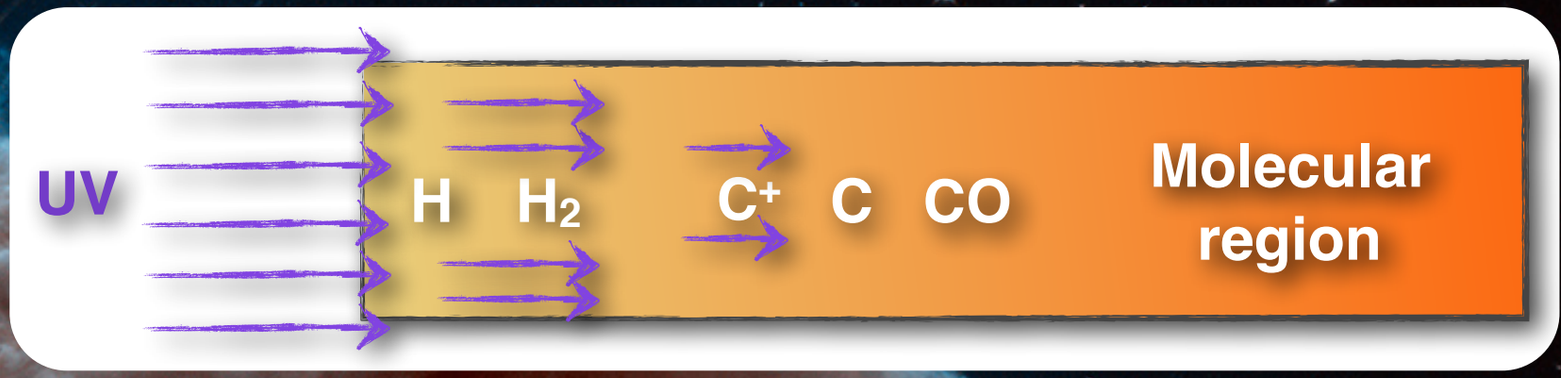
Hennebelle et al (2008)

The Meudon PDR code

Computes the atomic and molecular structure of ISM clouds

- Stationary
- One-dimensional





Processes included

- **UV radiative transfer:**
  - Absorption in molecular lines
  - Absorption in the continuum (dust)
  - 10000's of lines (including 30000 H_2 lines)
  - NLTE treatment of level populations
- **Chemistry :**
  - Several hundred chemical species
  - Several thousand chemical reactions
  - Photoionization / Photodissociation
  - Cosmic ray ionization
- **Thermal balance:**
  - Photoelectric effect
  - Chemical reactions
  - Cosmic rays
  - Atomic and molecular cooling

Outputs of the code

- **Local quantities :**
  - Abundance and excitation of species
  - Detailed heating and cooling rates
  - Radiation field energy density
  - Gas and grain temperatures, grain charge
  - Chemical reaction rates
- **Integrated quantities on the line of sight :**
  - Species column densities
  - Line intensities (H_2, CO, H_2O,…)
  - Absorption of the radiation field
  - Spectra

http://pdr.obspm.fr

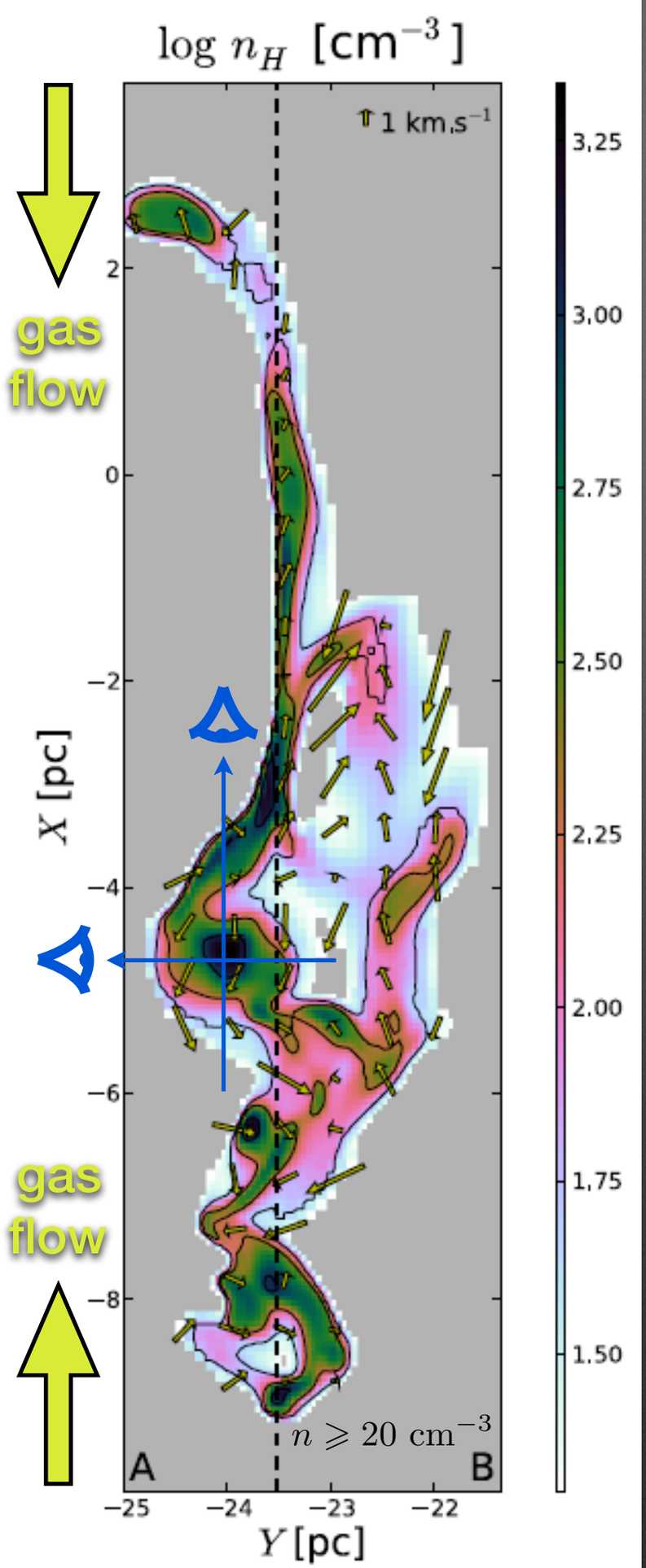
Le Bourlot et al. 1999
Le Petit et al. 2006
Goicoechea & Le Bourlot 2007
Gonzalez-Garcia et al. 2008
Le Bourlot et al. 2012
Bron 2014

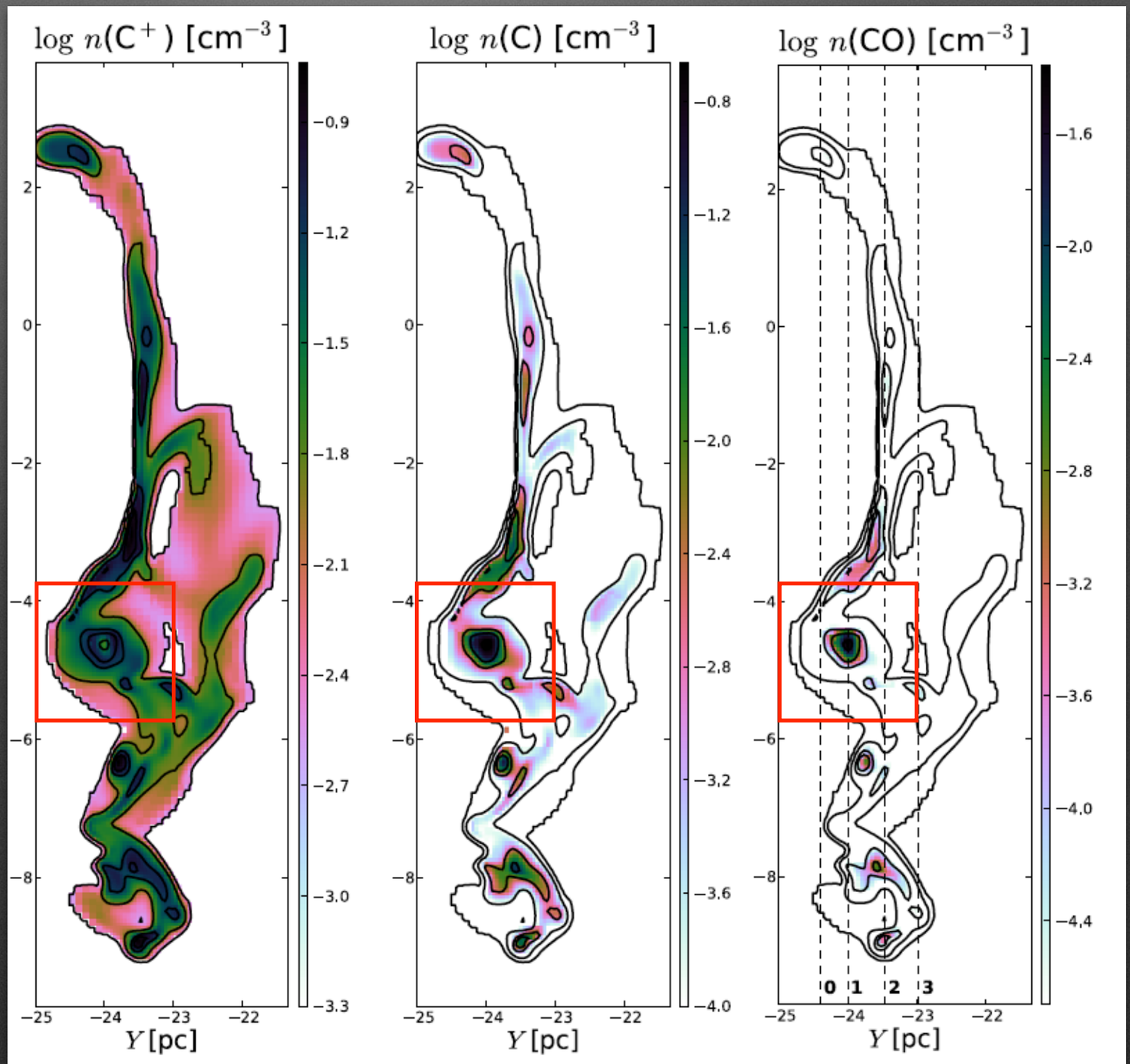
An example MHD-PDR post-processing

PDR code run on 1D density profiles above 20 cm^{-3} extracted along lines of sight either parallel to X or Y.

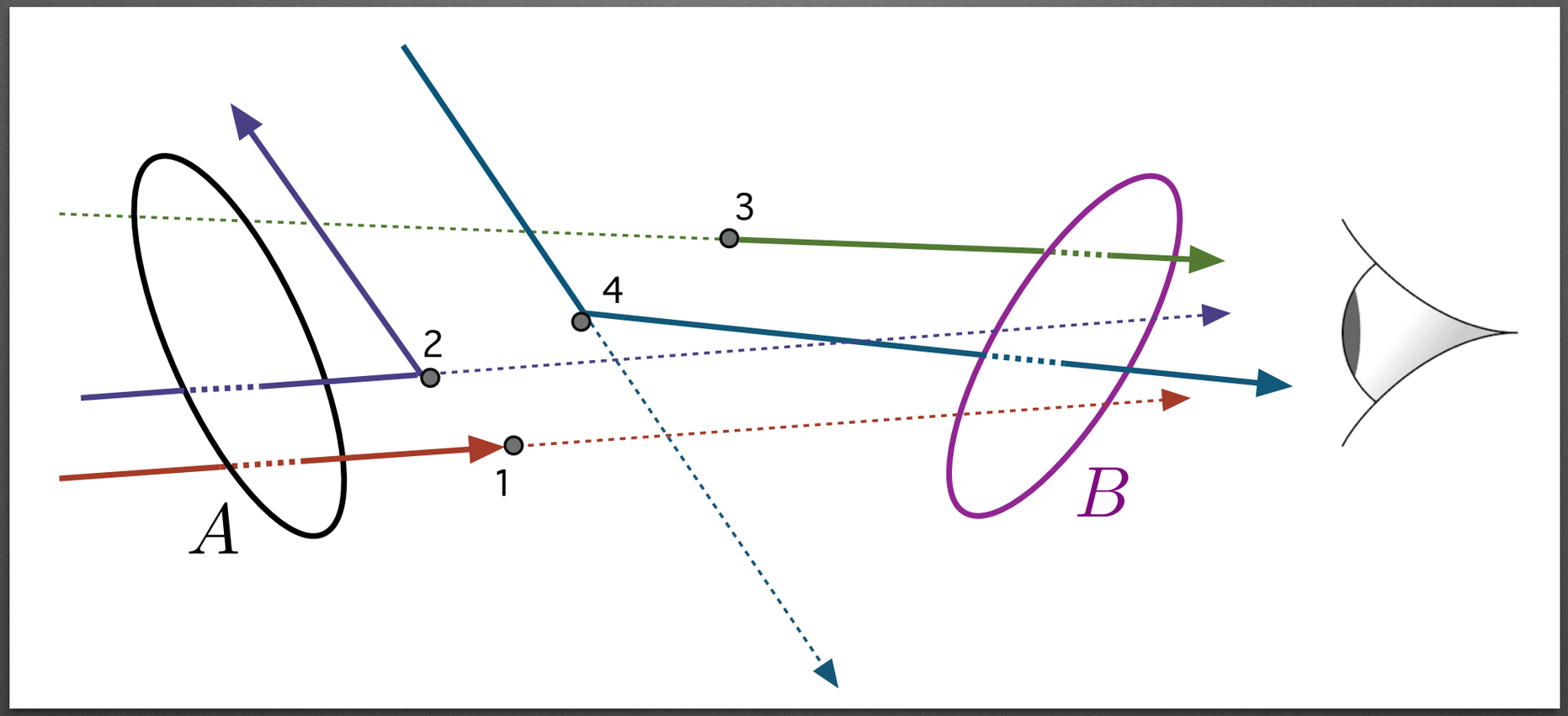
Outputs (temperature, chemical abundances) combined in 2D arrays.

Levrier et al. (2012)





Radiative Transfer



Absorption [1] Diffusion [2] Emission [3] Diffusion [4]

$$\boldsymbol{k}.\boldsymbol{\nabla} I_\nu\left(\boldsymbol{x},\boldsymbol{k}\right) = -\left[\kappa_\nu(\boldsymbol{x}) + \sigma_\nu(\boldsymbol{x})\right] I_\nu\left(\boldsymbol{x},\boldsymbol{k}\right) + \epsilon_\nu(\boldsymbol{x}) + \sigma_\nu(\boldsymbol{x}) J_\nu(\boldsymbol{x})$$

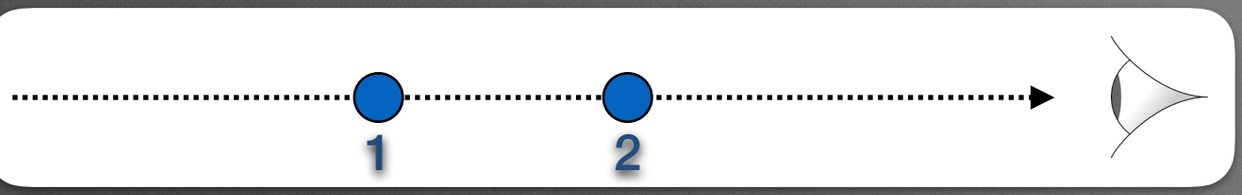
Highly non-linear coupling between matter and radiation

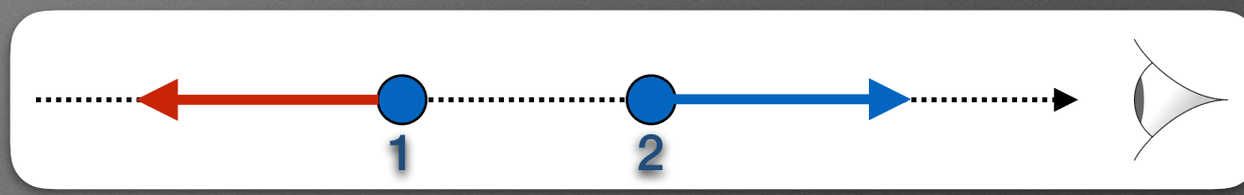
Solving radiative transfer with LVG methods

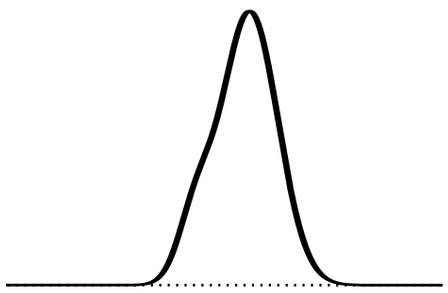
e.g. RADEX — Van der Tak et al. (2007)

http://home.strw.leidenuniv.nl/~moldata/radex.html

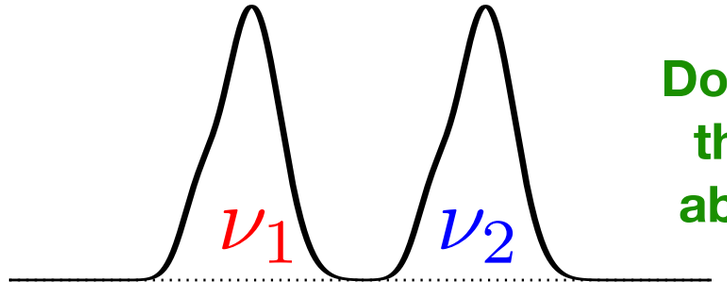
Photons may escape in velocity space







A photon emitted at (1) towards the observer may be absorbed at (2)



Doppler effect shifts the emission and absorption profiles

$$l = \frac{\sigma_T}{\boldsymbol{k}.\boldsymbol{\nabla}\left(\boldsymbol{k}.\boldsymbol{u}\right)}$$

Thermal line width

Local velocity

Scale over which $\delta u_{\mathrm{LOS}} \simeq \sigma_T$

Shu, « The physics of astrophysics, Vol. 1 » (1991)

Large velocity gradient (LVG) approximation

$l \ll L$

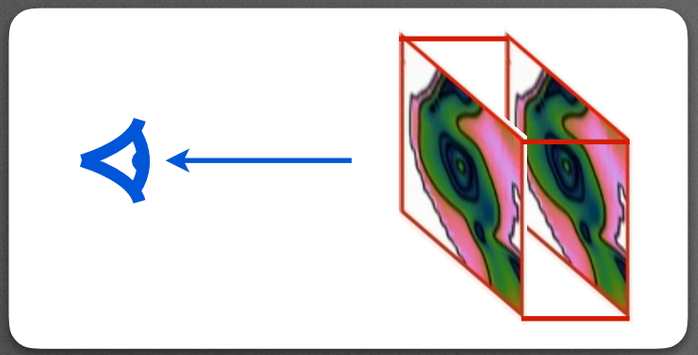
Typical size scale

Gas at a given position emits around $\nu = \nu_0 \left(1 + \frac{\boldsymbol{k}.\boldsymbol{u}}{c}\right)$

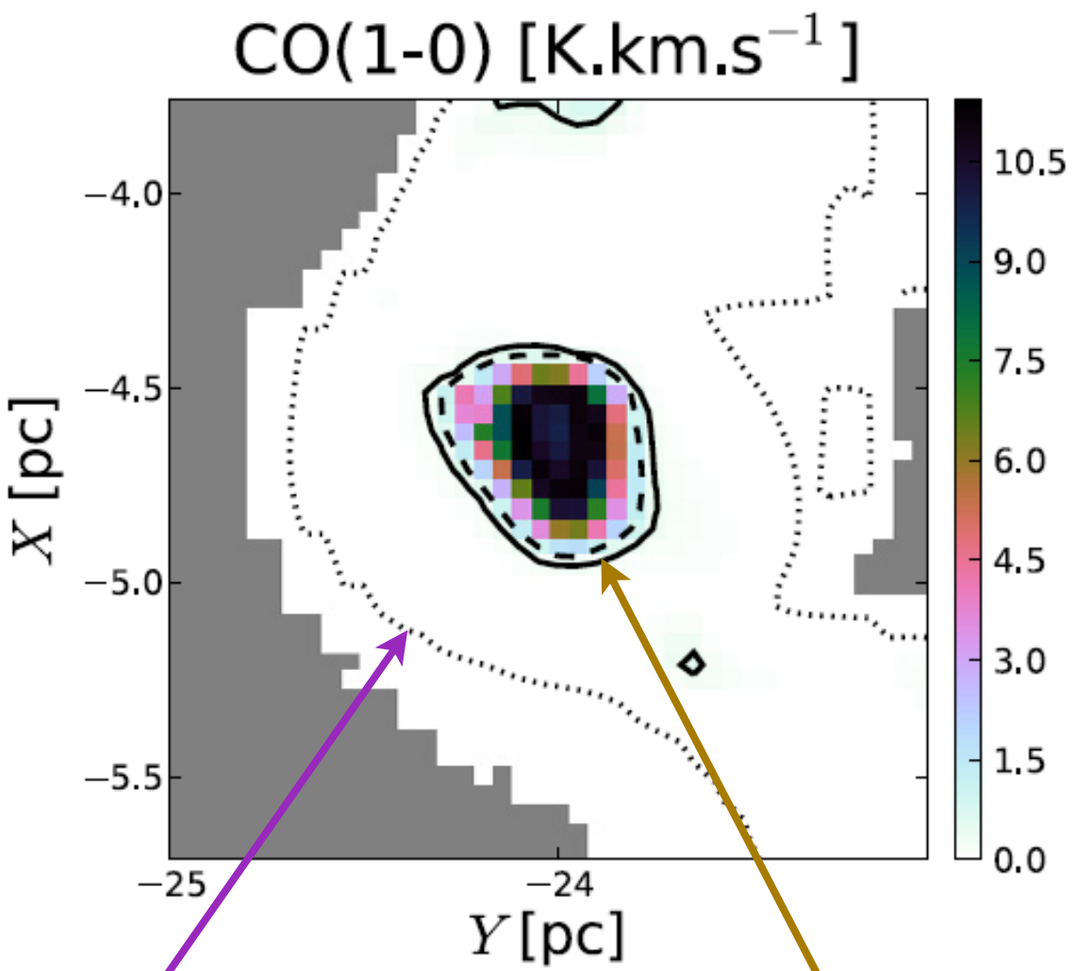
For pure expansion or contraction dynamics, the position-frequency relation is one-to-one along each line of sight

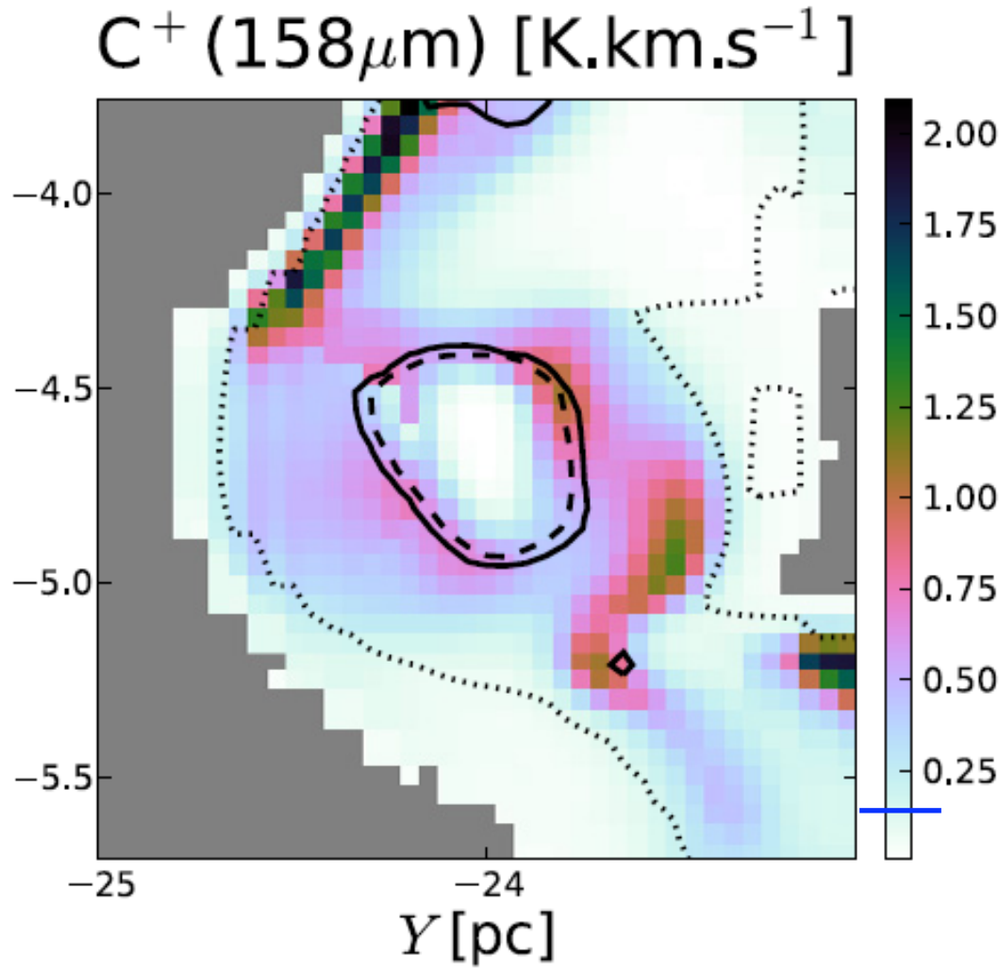
Careful with line overlap !

Simulated emission maps



Radiative transfer with RADEX (LVG approximation)





$f_{\mathrm{H_2}} = 1/2$

$W_{\mathrm{CO}} = 0.4$ K.km.s^{-1}

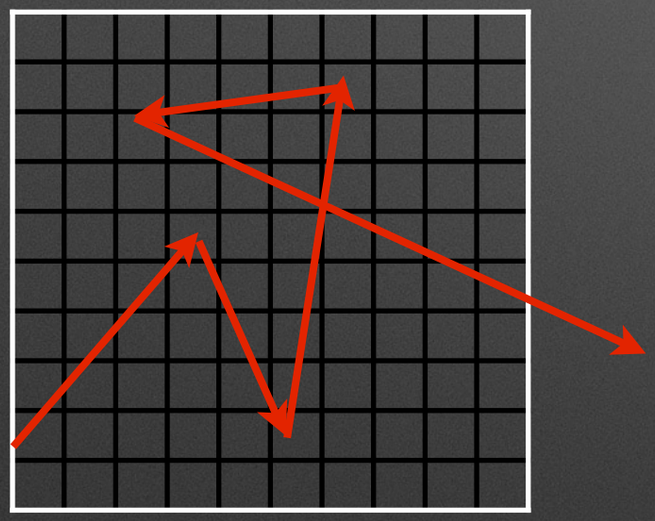
$\sigma_{\mathrm{CII}} = 0.1 - 0.2$ K.km.s^{-1}

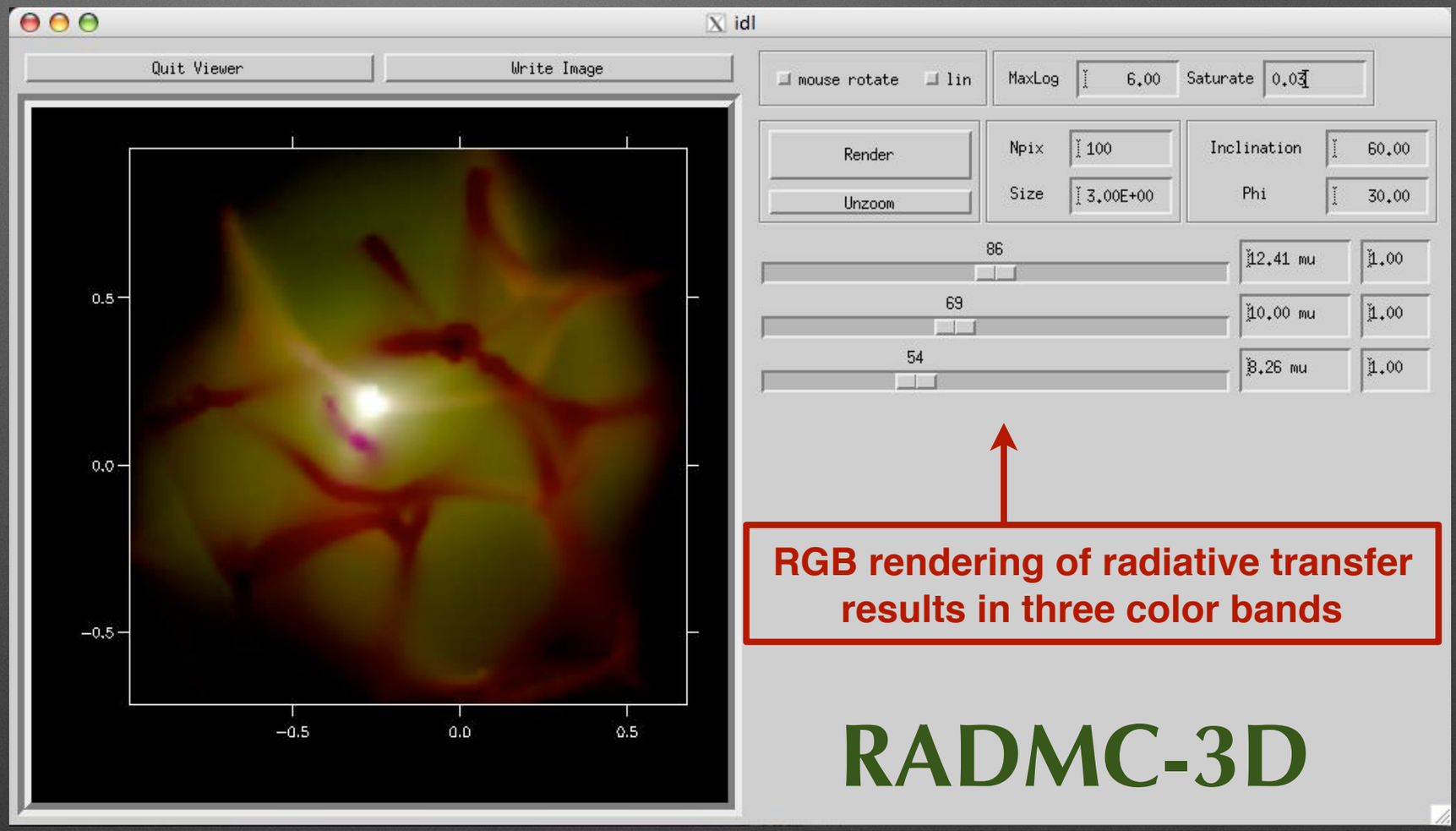
Velusamy et al. (2010)

Solving radiative transfer with Monte-Carlo methods

(Many) photons launched at « random » and tracked

- **Length and direction of next free-flight**
- **Type of interaction ending the free-flight (absorption or diffusion)**





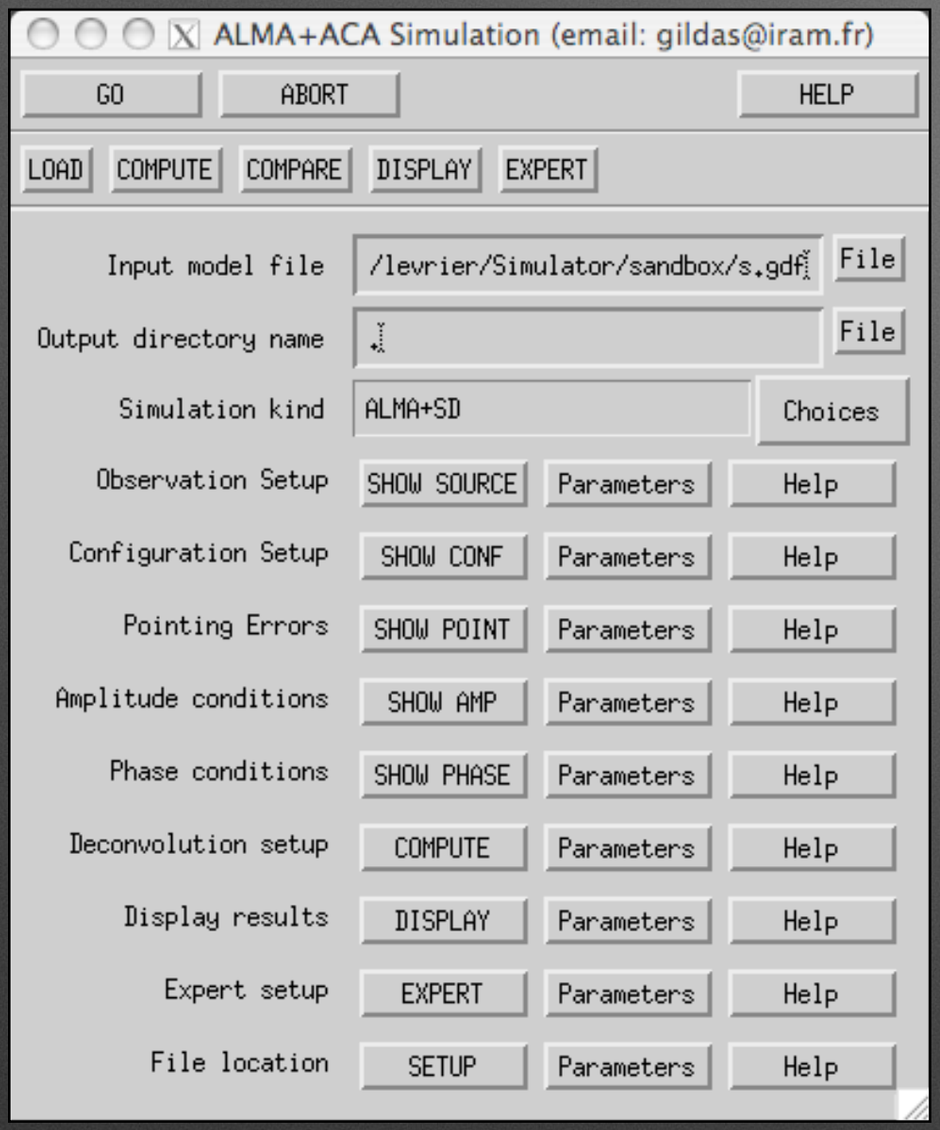
www.ita.uni-heidelberg.de/~dullemond/software/radmc-3d/

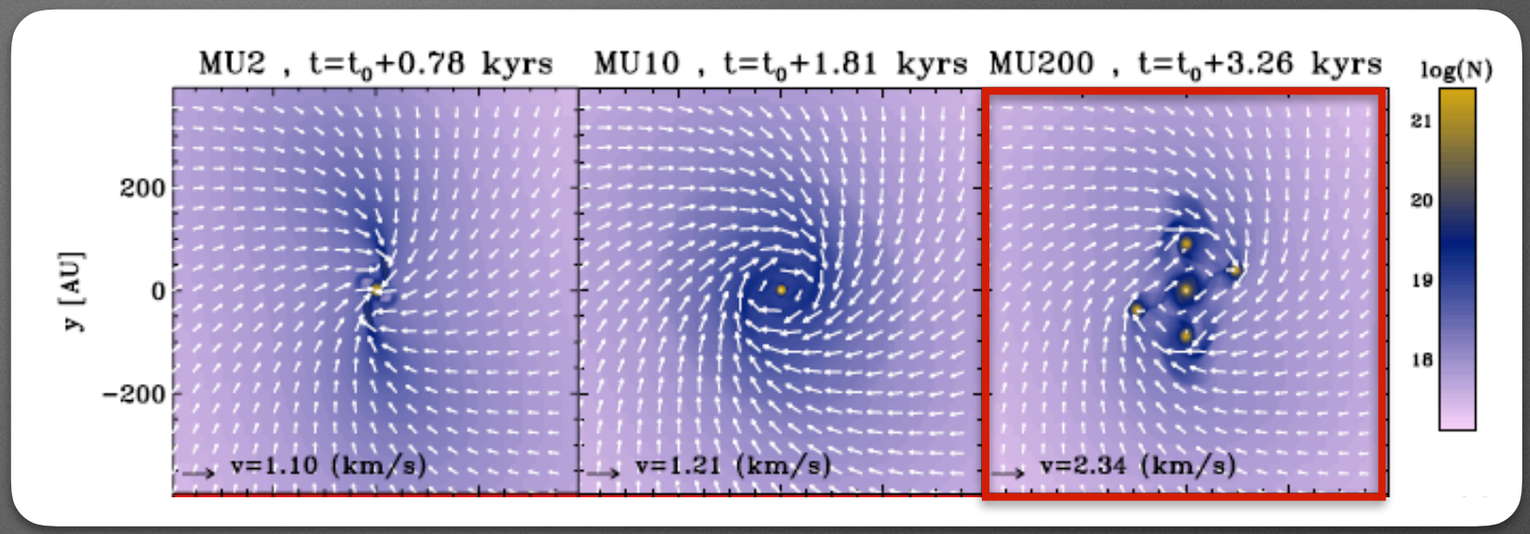
- Easy to understand, implement and upgrade with new microphysics
- Works equally well in any geometry
- Inherently noisy
- May require large computing resources

Simulated ALMA observations

ALMA Simulator in GILDAS applied on prestellar core simulations

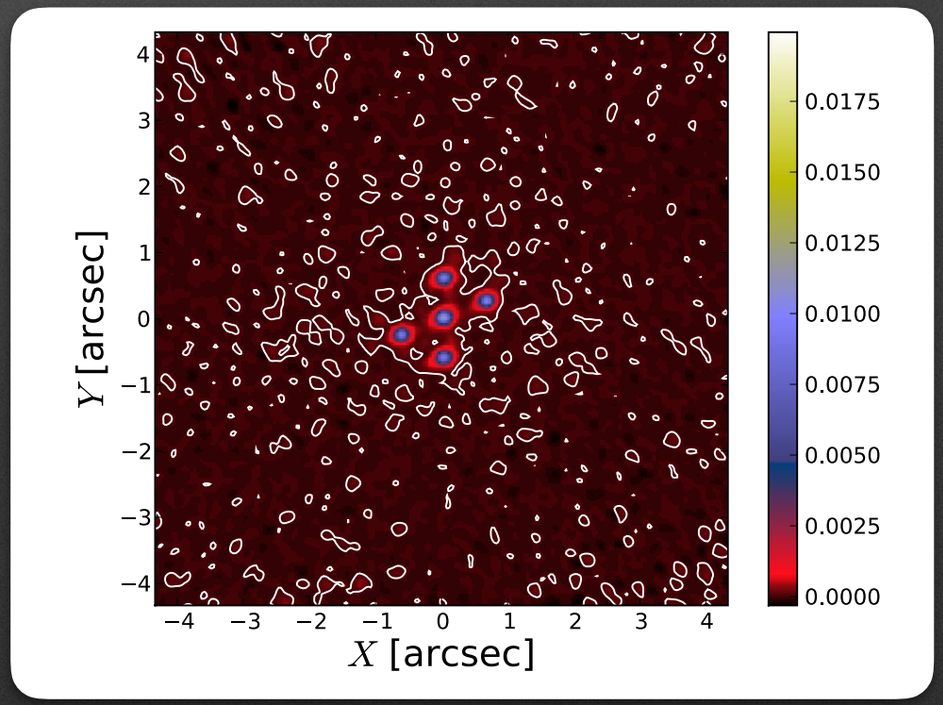
Commerçon et al. 2012





Dust emission maps with RADMC-3D

Simulated observations with GILDAS



iram
Institut de Radioastronomie Millimétrique

ALMA
ATACAMA LARGE MILLIMETER ARRAY

www.iram.fr/IRAMFR/GILDAS

RADMC-3D on STARFORMAT

STARFORMAT allows online RADMC-3D computation on MHD simulation results

Calculate radiation transfer on this clump thanks to RADMC-3D

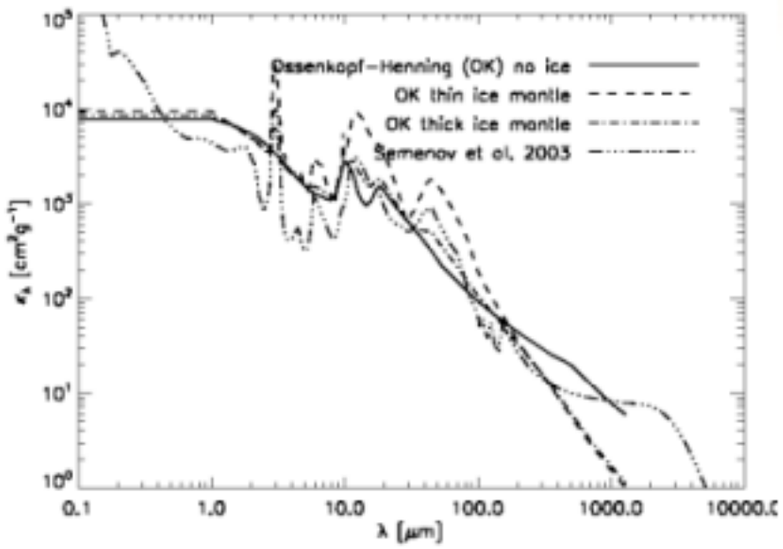
or Extract a subset of clump data from the simulation

What do you want to calculate?

- ◯ an image
- ◯ a SED

Which dust opacity model do you want to use?

- ◯ No ice
- ◯ Thin ice
- ◯ Thick ice
- ◯ Silicate
- ◯ Semenov



Clump box size: 1,76 pc (50,00 pc for the whole simulation)

Centered on: X 26,025 (pc) Y 26,953 (pc) Z 28,076 (pc)

Precision L_{max}: 10 corresponding to a resolution of 0.048 pc/cell
(maximum L_{max} allowed for this size of extraction: 12)

E-mail address (to receive a link to download the results):

Extract Reset Cancel

The Meudon PDR database search

Forward modeling is so 2012

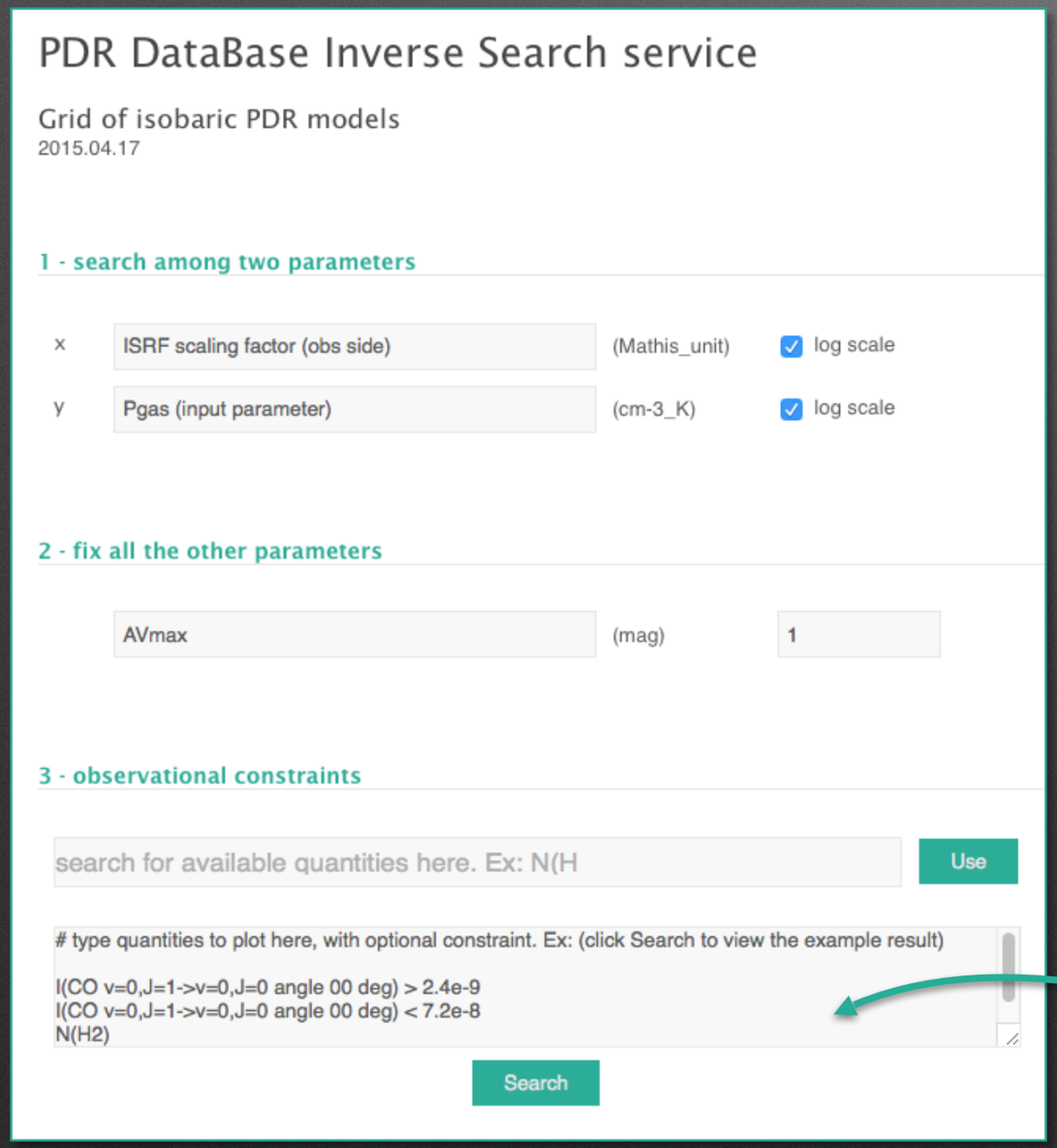
Grids of PDR models may be searched on ~10 input parameters :

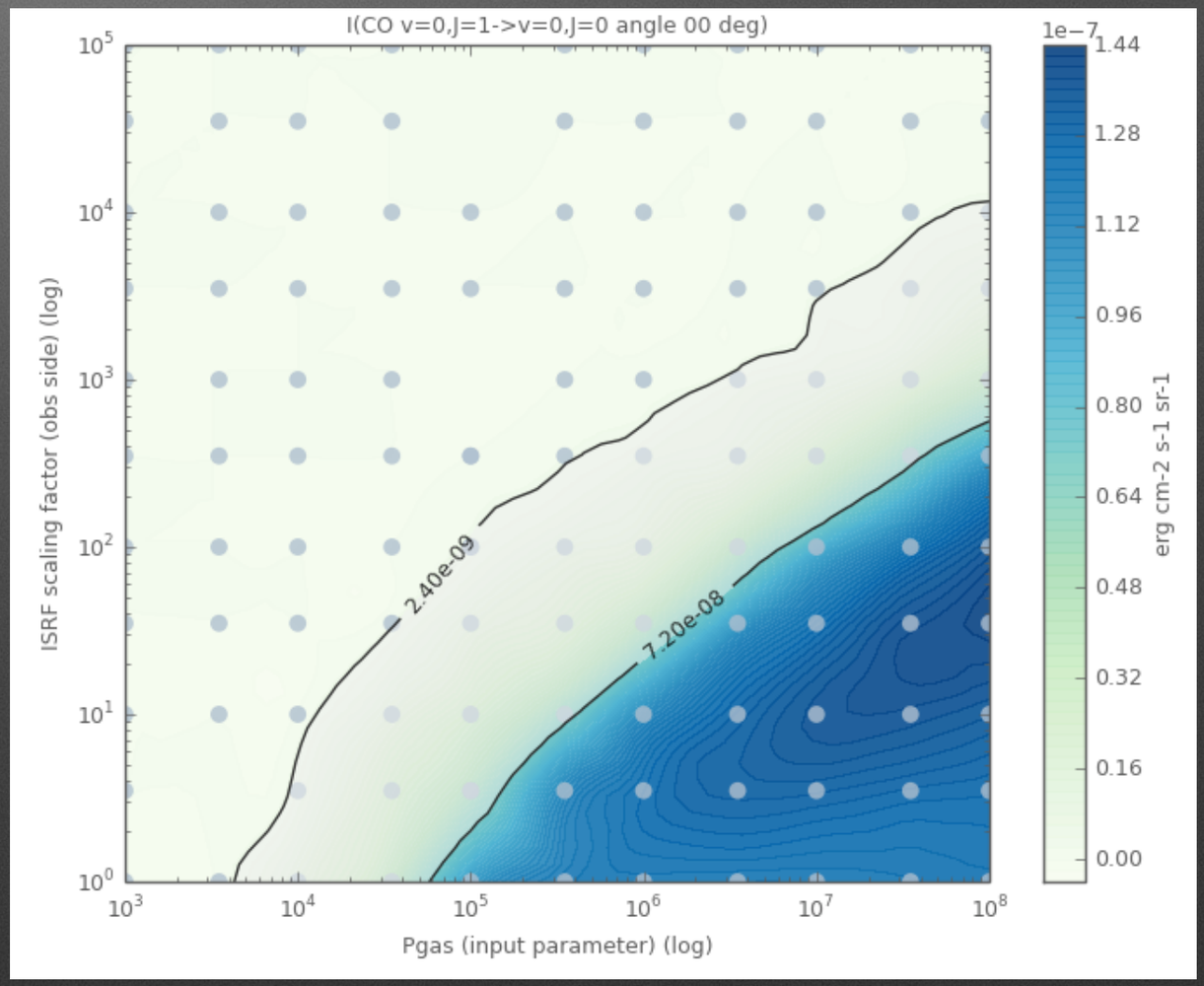
« What is the CO(15-14) intensity in a cloud of density $n_H = 10^4$ cm^{-3}, $G_0 = 1000$? »

The true challenge is querying databases on output parameters

Requires searching on some 150,000 output parameters of PDR models :

« Which PDR models have CII[158 µm] line larger than 10^{-7} erg/s/cm^2/sr and … and … and … »





Queries on

- line intensities (several ten thousands)
- column densities and levels populations

(D. Languignon, F. Le Petit, E. Bron, B. Godard)

Ye olden days of inverse problems

Example : Interpretation of FUSE observations towards HD 102065

Nehmé et al. (2008)

Aims. We model a diffuse molecular cloud present along the line of sight to the star HD 102065. We compare our modeling with observations to test our understanding of physical conditions and chemistry in diffuse molecular clouds.
Methods. We analyze an extensive set of spectroscopic observations which characterize the diffuse molecular cloud observed toward HD 102065. Absorption observations provide the extinction curve, H_2, C I, CO, CH, and CH^+ column densities and excitation. These data are complemented by observations of C^+, CO and dust emission. Physical conditions are determined using the Meudon PDR model of UV illuminated gas.
Results. We find that all observational results, except column densities of CH, CH^+ and H_2 in its excited ($J \geq 2$) levels, are consistent with a cloud model implying a Galactic radiation field ($G \sim 0.4$ in Draine's unit), a density of 80 cm^{-3} and a temperature (60–80 K) set by the equilibrium between heating and cooling processes. To account for excited ($J \geq 2$) H_2 levels column densities, an additional component of warm (~250 K) and dense ($n_H \geq 10^4$ cm^{-3}) gas within 0.03 pc of the star would be required. This solution reproduces the observations only if the ortho-to-para H_2 ratio at formation is ~1. In view of the extreme physical conditions and the unsupported requirement on the ortho-to-para ratio, we conclude that H_2 excitation is most likely to be accounted for by the presence of warm molecular gas within the diffuse cloud heated by the local dissipation of turbulent kinetic energy. This warm H_2 is required to account for the CH^+ column density. It could also contribute to the CH abundance and explain the inhomogeneity of the CO abundance indicated by the comparison of absorption and emission spectra.

	X^{mod}	X^{obs}	σ_{obs}
$N(CO)/N(H_2)$	1.5 (−7)	1.6 (−7)	$\pm^{0.2\,(-7)}_{0.15\,(-7)}$
$N(C\,I)/N_H$	5.8 (−7)	6.0 (−7)	±1.5 (−7)
$N(C\,I^*_{J=1})/N(C\,I)$	0.17	0.16	±0.07
$N(C\,I^{**}_{J=2})/N(C\,I)$	0.03	0.024	±0.01
$f_{H_2} = \frac{2N(H_2)}{N(H)+2N(H_2)}$	0.9	0.69	±0.12
$N(H_2^o)/N(H_2^p)$	0.73	0.7	±0.12
$I(C^+)$ (erg/s cm^2 sr)	2.0 (−6)	2.8 (−6)	±0.85 (−6)
$N(CH)/N(H_2)$	8.4 (−9)	1.85 (−8)	±0.3 (−8)
$N(CN)/N(H_2)$	1.2 (−10)	<1.5 (−9)	
$N(C_2)/N(H_2)$	3.6 (−8)	<3.5 (−8)	
$N(CO_{J=0})/N(H_2)$	9.0 (−8)	9.6 (−8)	$\pm^{1.4\,(-8)}_{1.7\,(-8)}$
$N(CO_{J=1})/N(H_2)$	5.1 (−8)	6.2 (−8)	$\pm^{1.5\,(-8)}_{1.2\,(-8)}$
$N(CO_{J=2})/N(H_2)$	3.7 (−9)	<7.3 (−9)	

Harvard computers, circa 1890

The future is now

Plot axis

x: nH (input parameter) log scale

y: ISRF scaling factor (observer side) log scale

Fixed axis

AVmax 0.5

Axis constraints

Add ex: X-ray power law slope > -1

N(H2) > 3.1E20
N(H2) < 3.7E20
N(C) > 3.0E14
N(C) < 5.0E14
I(C+ El=2P,J=3/2->El=2P,J=1/2) > 1.95E-6
I(C+ El=2P,J=3/2->El=2P,J=1/2) < 3.65E-6

Plot

Query :

3.1E20 < N(H_2) < 3.7E20
3.0E14 < N(C) < 5.0E14
1.9E-6 < I(C^+, 158 µm) < 3.6E-6
62 < T01 < 72

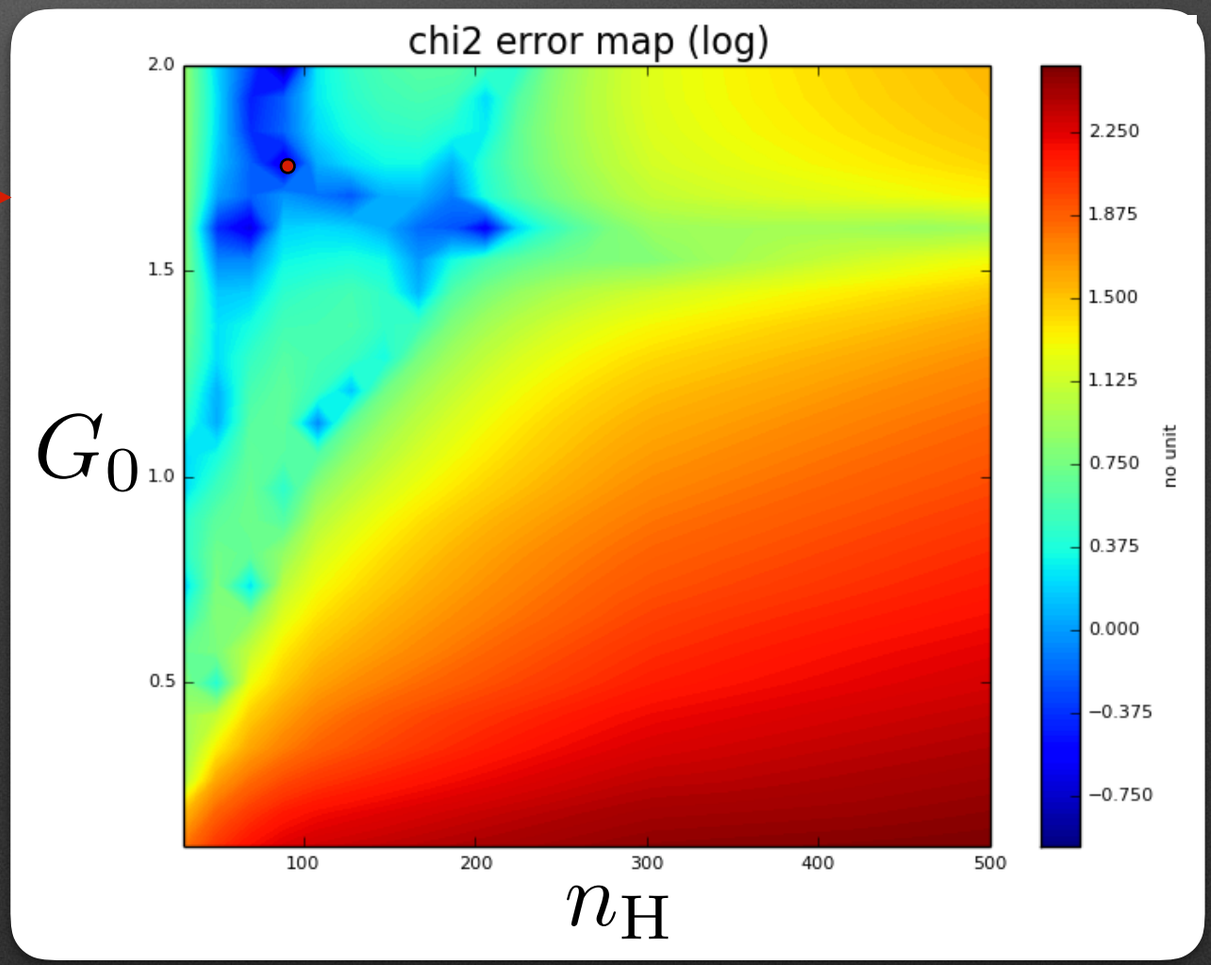
① select what you are looking for

Example : density & UV radiation field

② fix some quantities

Example : size of the cloud (A_V)

③ Enter the observed quantities as constraints for the search



Results :

- **n_H ~ 100 cm^{-3}**
- **G_0 ~ 1.7 Mathis**

Online codes

Interpretation of detailed observations (many constraints) requires to launch hundreds models
PDR code & Shock code may require several tens minutes to several days of computation for 1 run

PDL Standard (C.-M. Zwölf)

- Description of input parameters
- Relations between parameters
- Validity ranges for parameters
- Interoperability between services

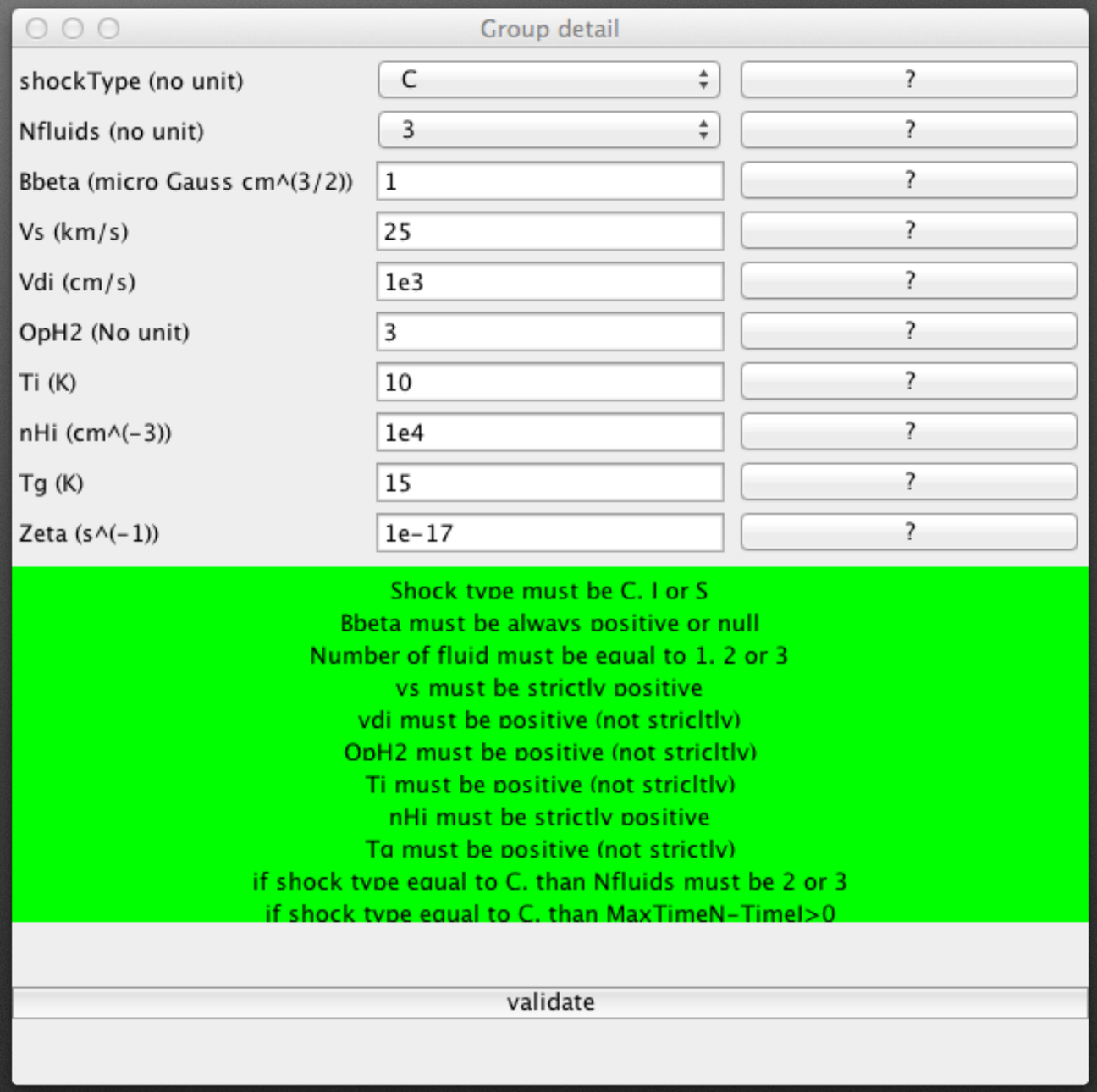
Architecture (C.M. Zwölf, J.F. Rabasse)

- PDL server : job management
- Access to Paris Observatory computing power
- For now Paris-Durham shock code
- PDR code will follow

User friendly

- Follow job online
- Email at job completion

Paris-Durham shock code web interface



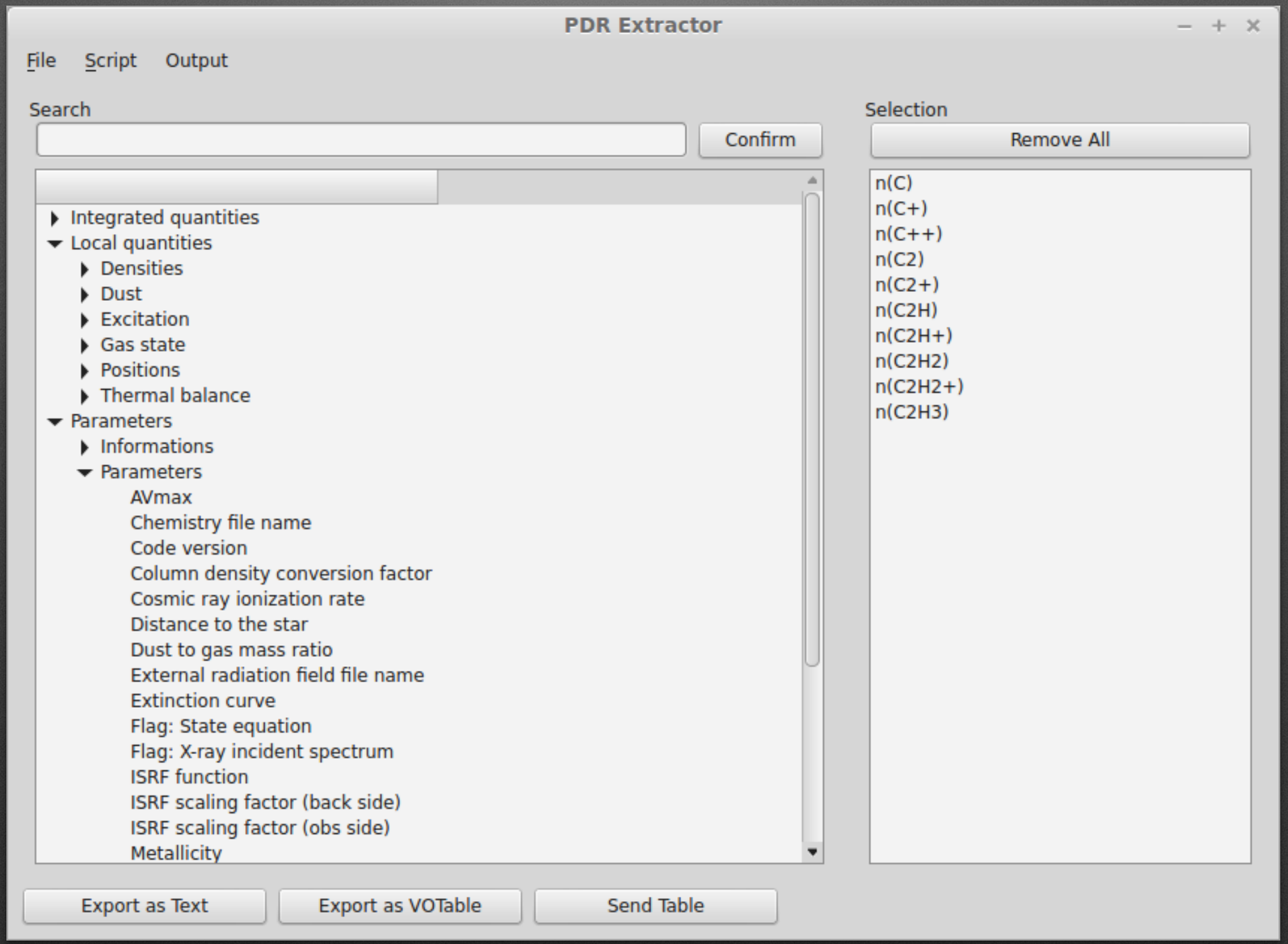
A. Gusdorf

Analysis tools

Data extraction tool

- New data format : HDF5
- New data extraction tool
- VO compatible (VO-Table & SAMP)

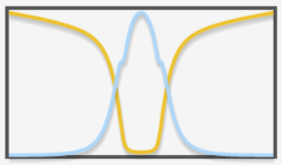
TOPCAT



Analysis tools

Chemical network analyzer

Control panel | Physical conditions



Temperature n(+CO)

Log x : ☐ **Log y :** ☐

AV : 5.0501e-1

n(CO) = 5.04e-13 cm-3

Species

CO

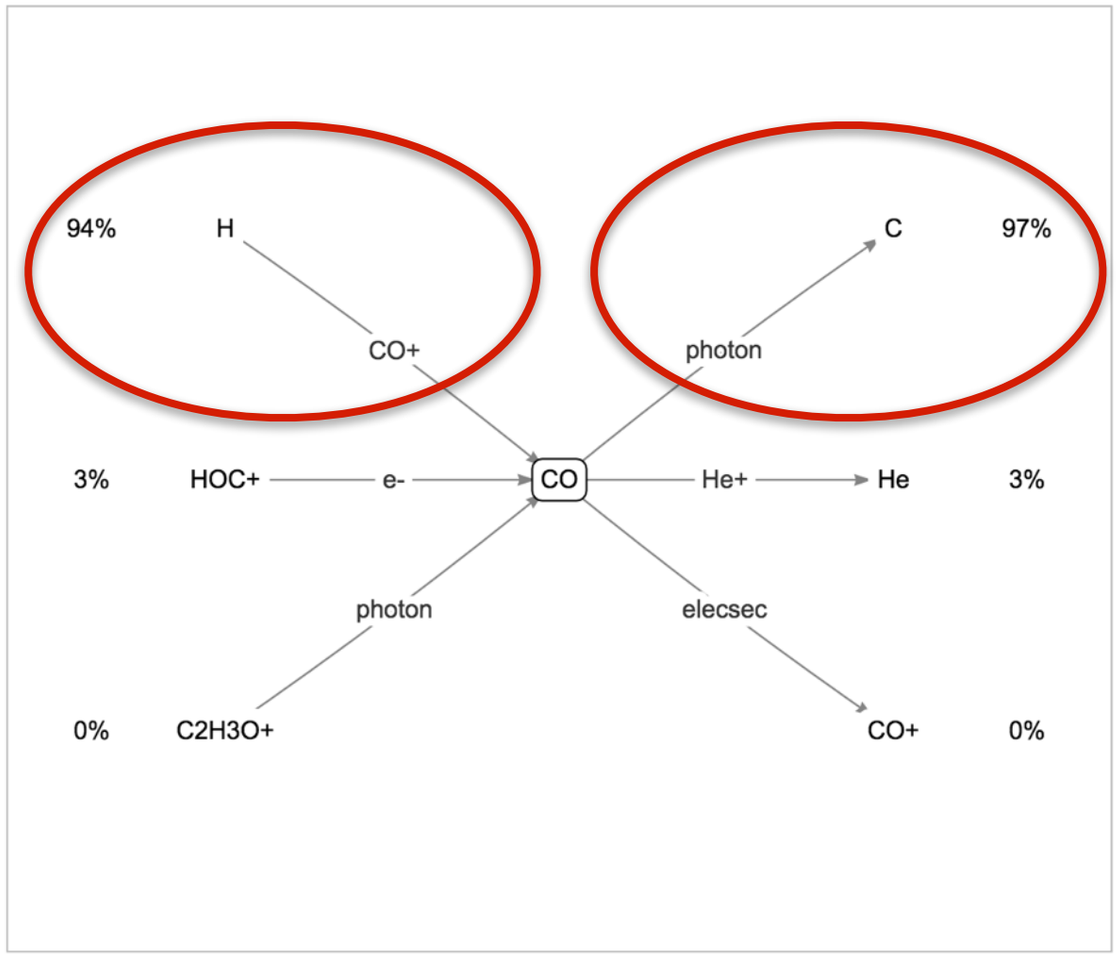
back

Gas ☑ **Grains** ☐

Gas conditions

nH	1.0e-1	cm-3
nd(e-)	-1.4e-8	cm-3
Xray	6.5e-25	cm-2 s-1
Tg	1.3e+3	K
zeta	3.0e-16	s-1 / H2
ng(e-)	2.1e-3	cm-3
UV	2.0e+7	cm-2 s-1

2S_a1p0n1m*r1p0z3p1x0p0m1p0xray_c_30.hdf5



formation reactions

A + B → C + D	n(A) (cm-3)	n(B) (cm-3)	k	rate (cm-3 s-1)	freq (s-1)
$H + CO^+ \rightarrow CO + H^+$	9.33e-2	8.59e-14	7.50e-10	6.01e-24	1.19e-11
$HOC^+ + e^- \rightarrow H + CO$	3.32e-15	2.13e-3	2.56e-8	1.81e-25	3.59e-13
$C_2H_3O^+ + photon \rightarrow CO + CH_3^+$	1.05e-31			3.43e-41	6.80e-29

destruction reactions

A + B → C + D	n(A) (cm-3)	n(B) (cm-3)	k	rate (cm-3 s-1)	freq (s-1)
$CO + photon \rightarrow C + O$	5.04e-13			6.19e-24	1.23e-11
$CO + He^+ \rightarrow He + O + C^+$	5.04e-13	2.72e-4	1.50e-9	2.06e-25	4.08e-13
$CO + elecsec \rightarrow CO^+ + e^-$	5.04e-13			2.35e-55	4.66e-43

Conclusions

Modeling the ISM is an incredibly complex problem

- Numerous physico-chemical processes
- Large dynamic range
- Coupling of scales

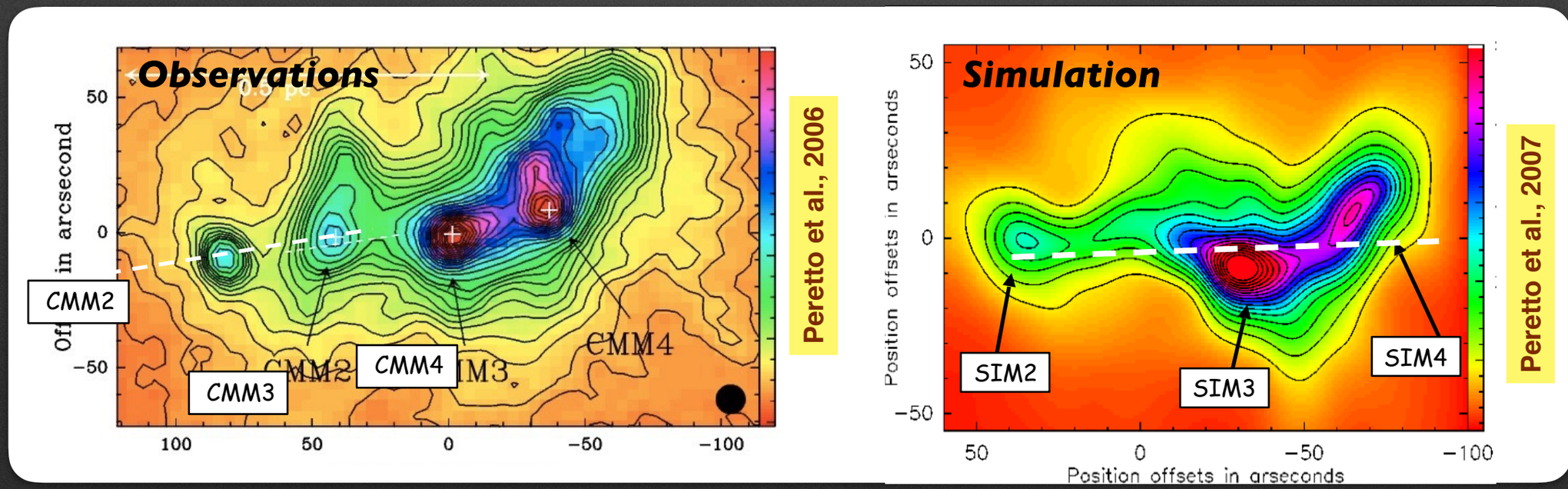
Possible approaches

- Detailed direct numerical approach impossible
- Post-processing of MHD simulations (chemistry, radiative transfer, observations)
- Or actual coupling with simplified processes

The ISM platform

- Databases searchable on output results
- Code coupling
- Online codes

Towards new methods to interpret observational data



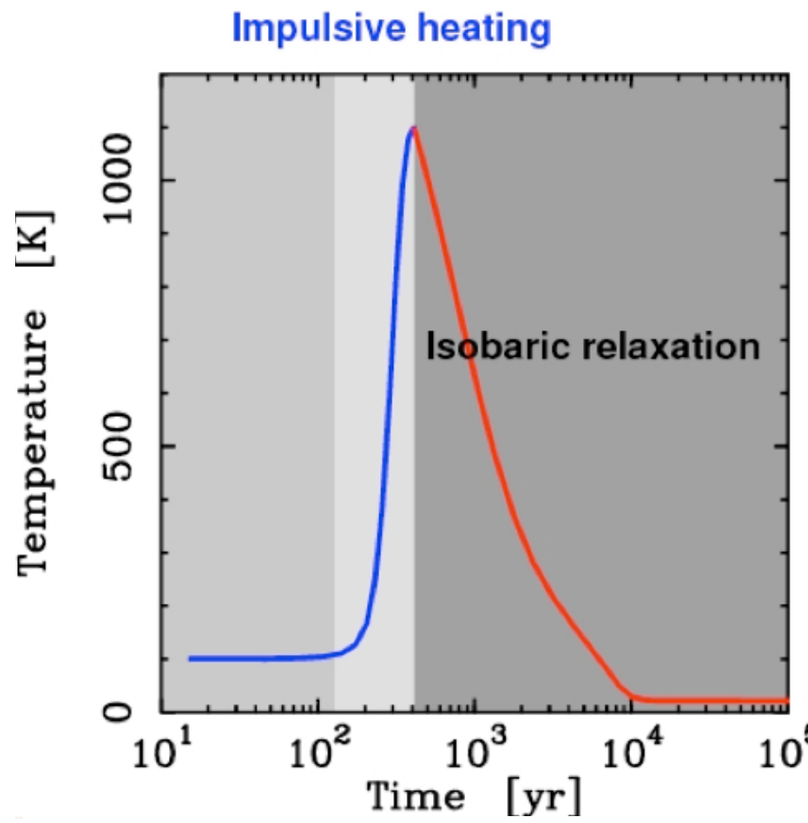
EXTRA SLIDES

The TDR model

Magnetized modified Burgers vortex

$$\omega_z(r) = \omega_0 \cdot \mathrm{e}^{-\frac{a}{4\nu\beta}\left[1-\mathrm{e}^{-\beta r^2}\right]}$$

a : Turbulent rate of strain



Joulain et al., 1998
Godard et al., 2009

Magnetized vortices:
~ 50 AU
~ 100 years lifetime

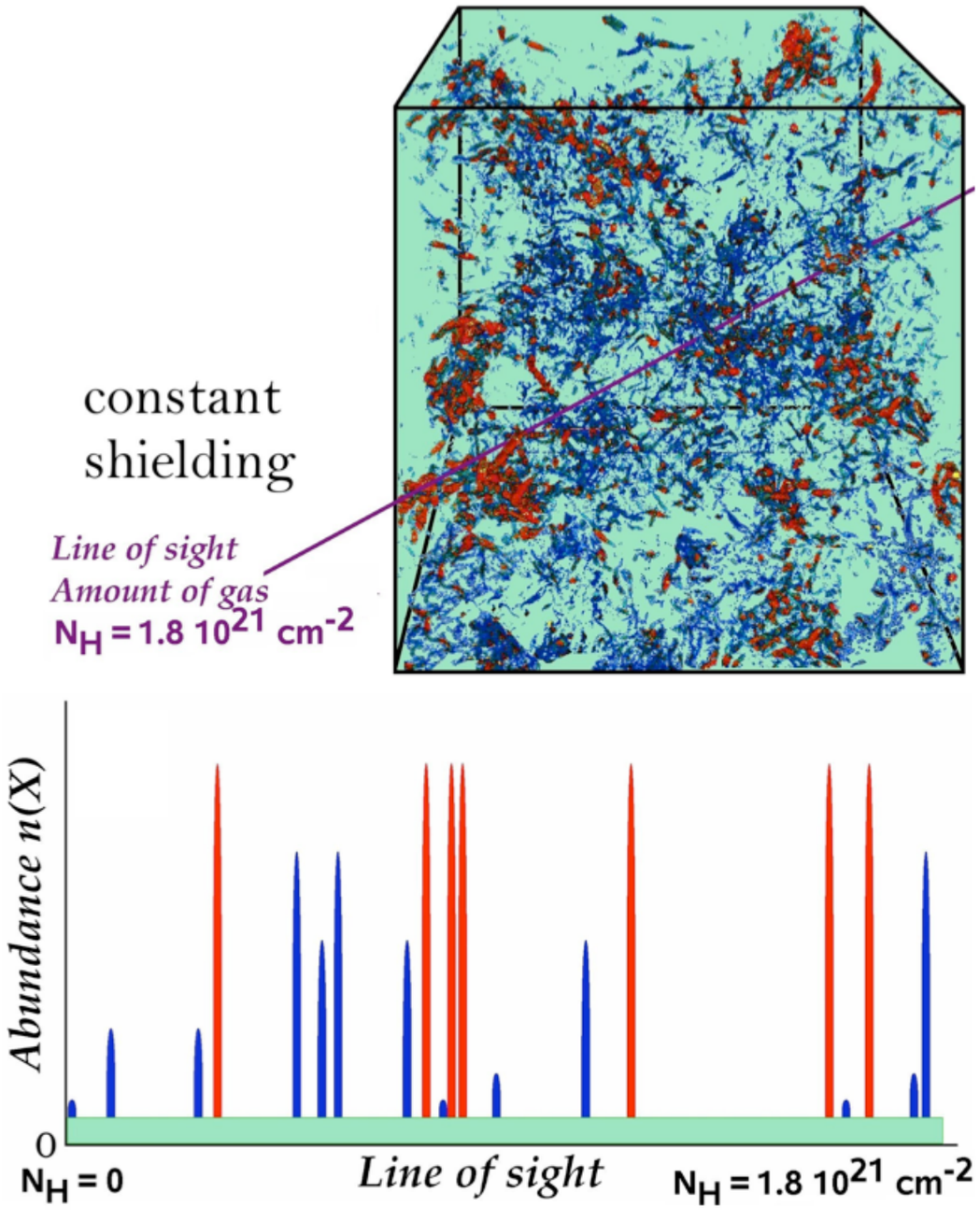
Dissipation leads to warm chemistry

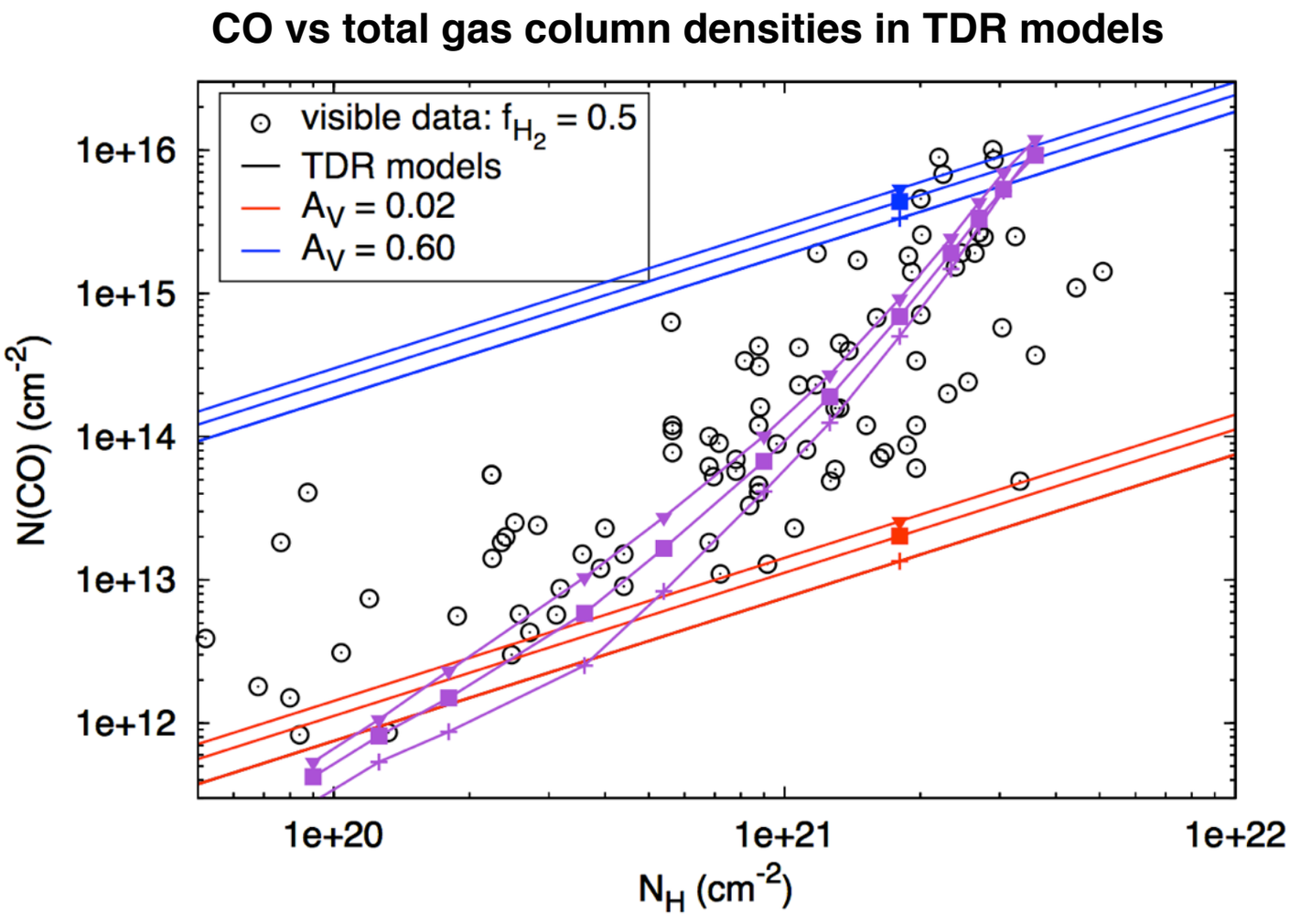
Thermal and chemical relaxation last up to 4.10^4 years

Free parameters a ; n_{H} ; A_{V}

3 phases : active and relaxing vortices, ambient medium

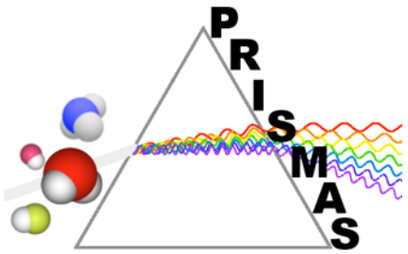
Chemical enrichment by turbulent dissipation



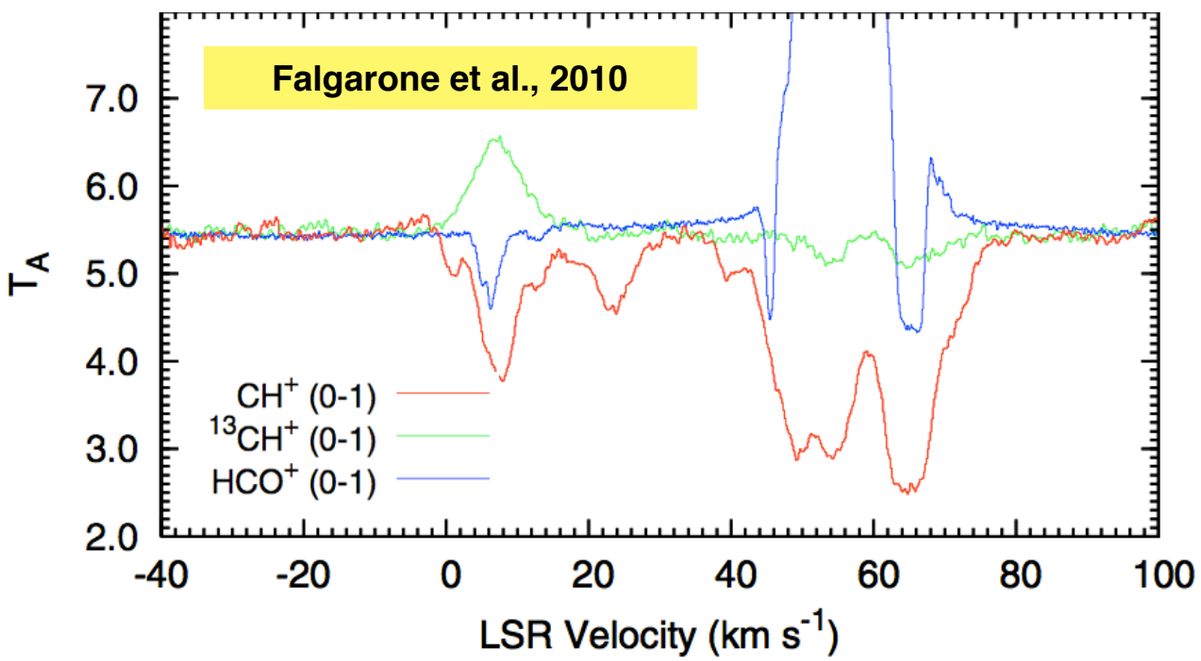


Godard et al. in prep

The CH^+ puzzle solved ?



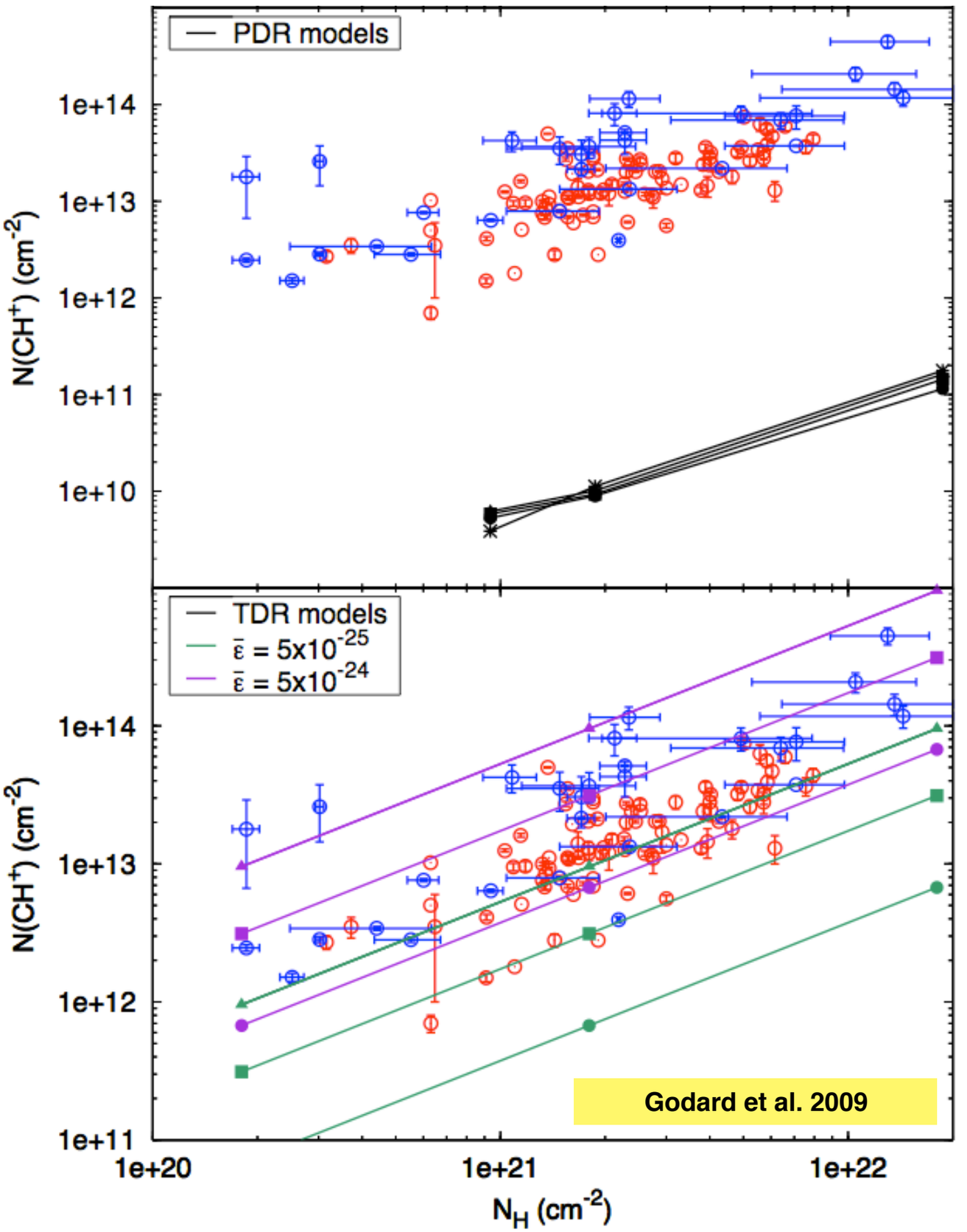
CH^+ absorption towards massive SF regions



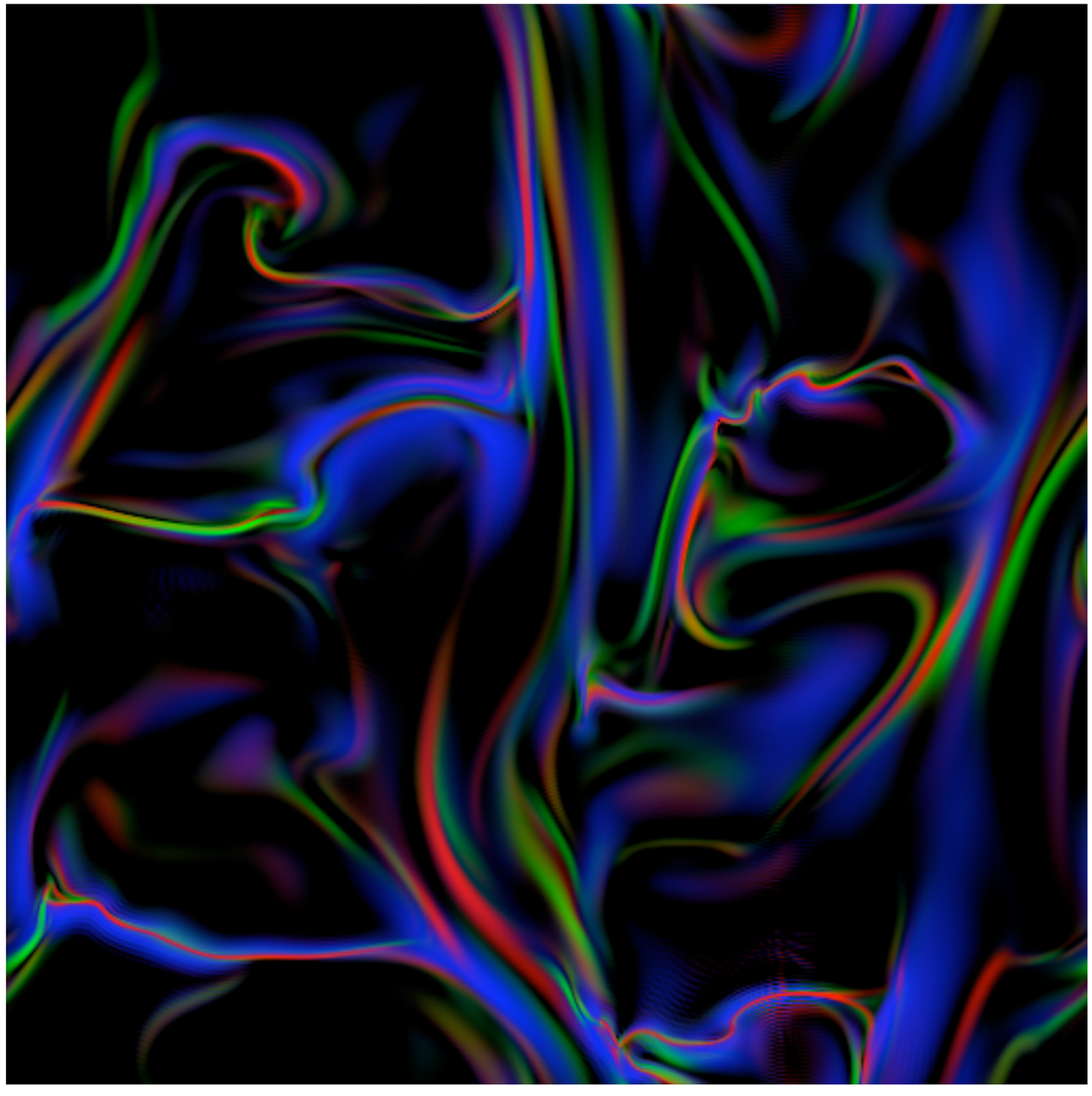
$$C^+ + H_2 \rightarrow CH^+ + H$$

HIGHLY ENDOTHERMIC (E/k=4640 K)

CH^+ abundances in PDR and TDR models



Dissipation processes



2D cut through a 512^3 incompressible turbulence simulation with the ANK code

Viscous heating

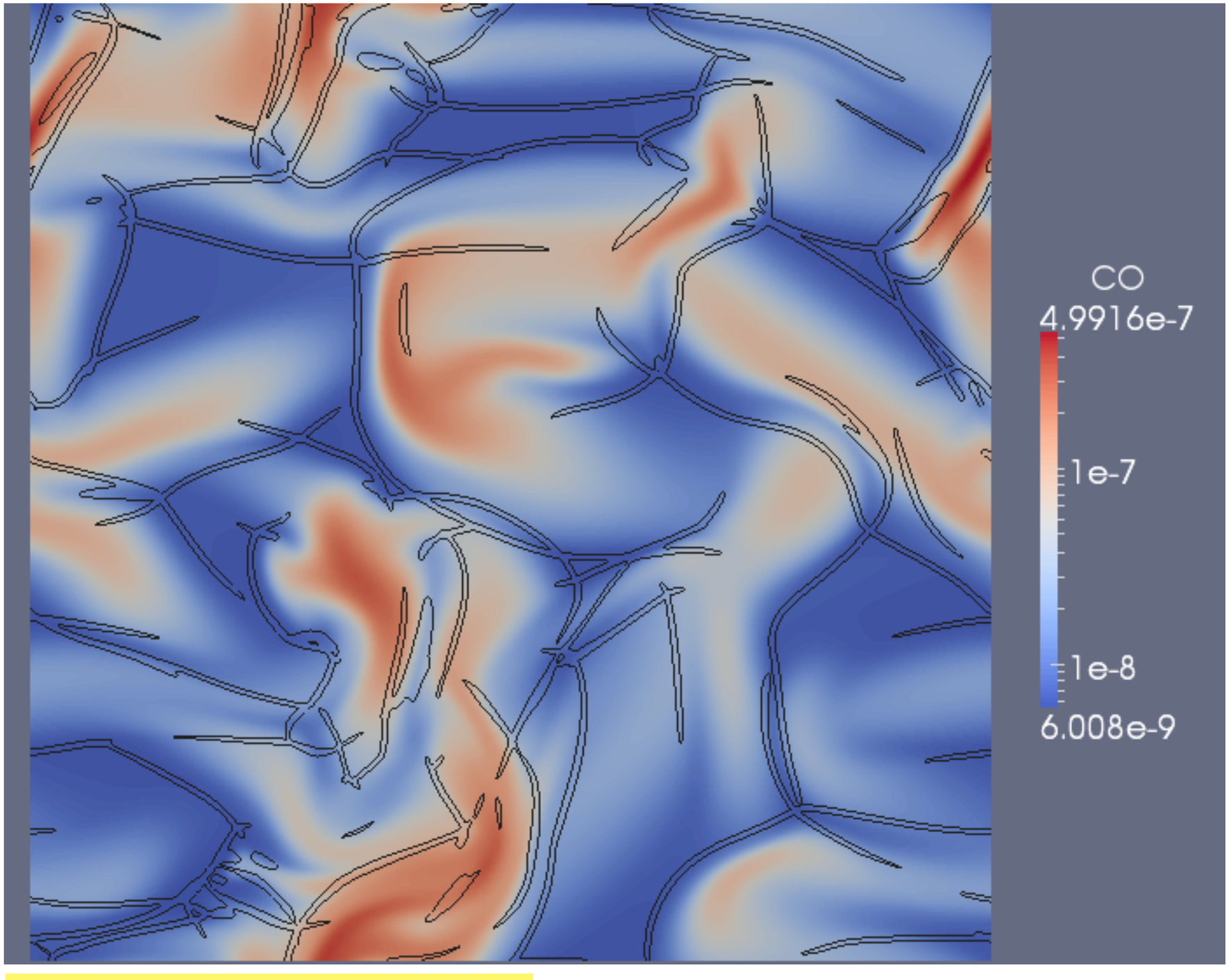
Ohmic heating

Ambipolar diffusion heating

Momferratos, Lesaffre, Falgarone, in prep.

Chemical enrichment in the wakes of shocks

<u>2D decaying turbulence simulation with chemical coupling</u>
- Colour scale : CO abundances
- Contours : Regions of high viscous heating



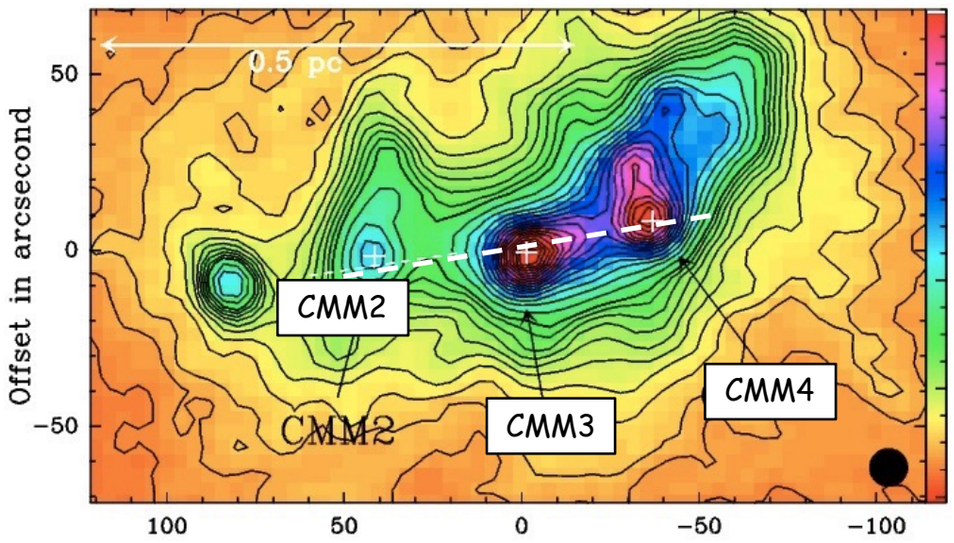
Lesaffre et al., in prep

A new path for interpreting observations

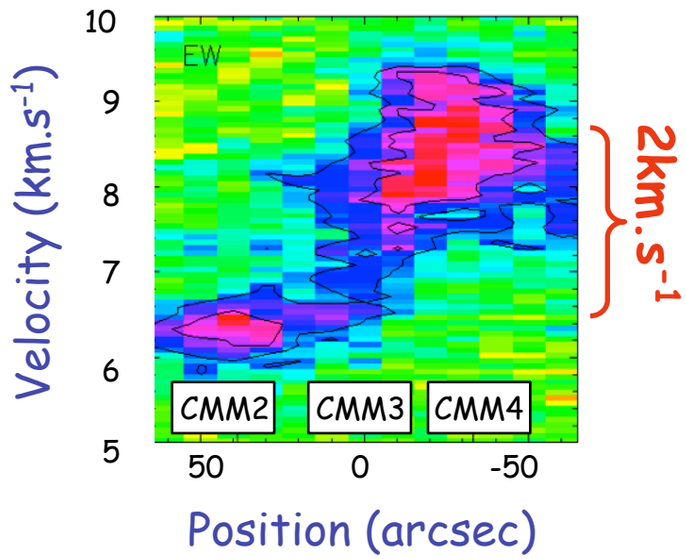
Observations with IRAM 30 m telescope

Peretto, André & Belloche, 2006

Continuum @ 1.2mm

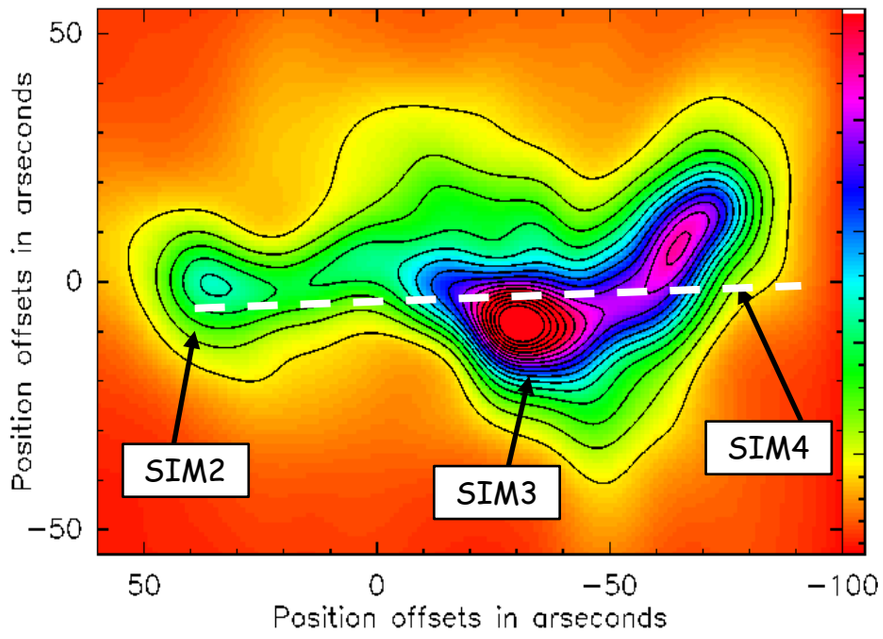


Position-Velocity diagram in the N_2H^+(101-012) line

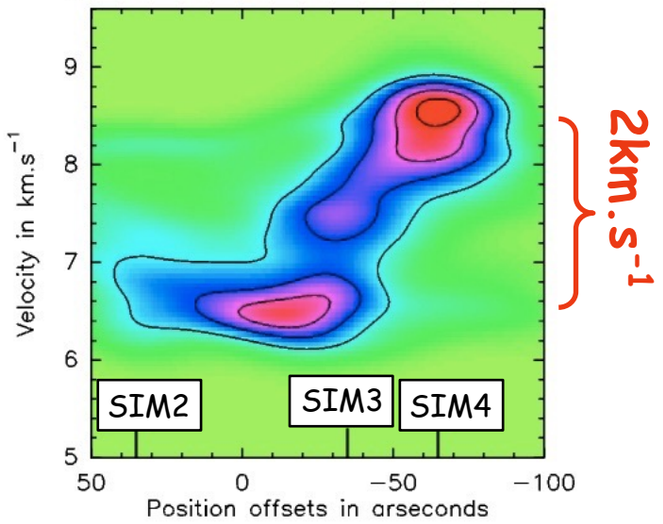


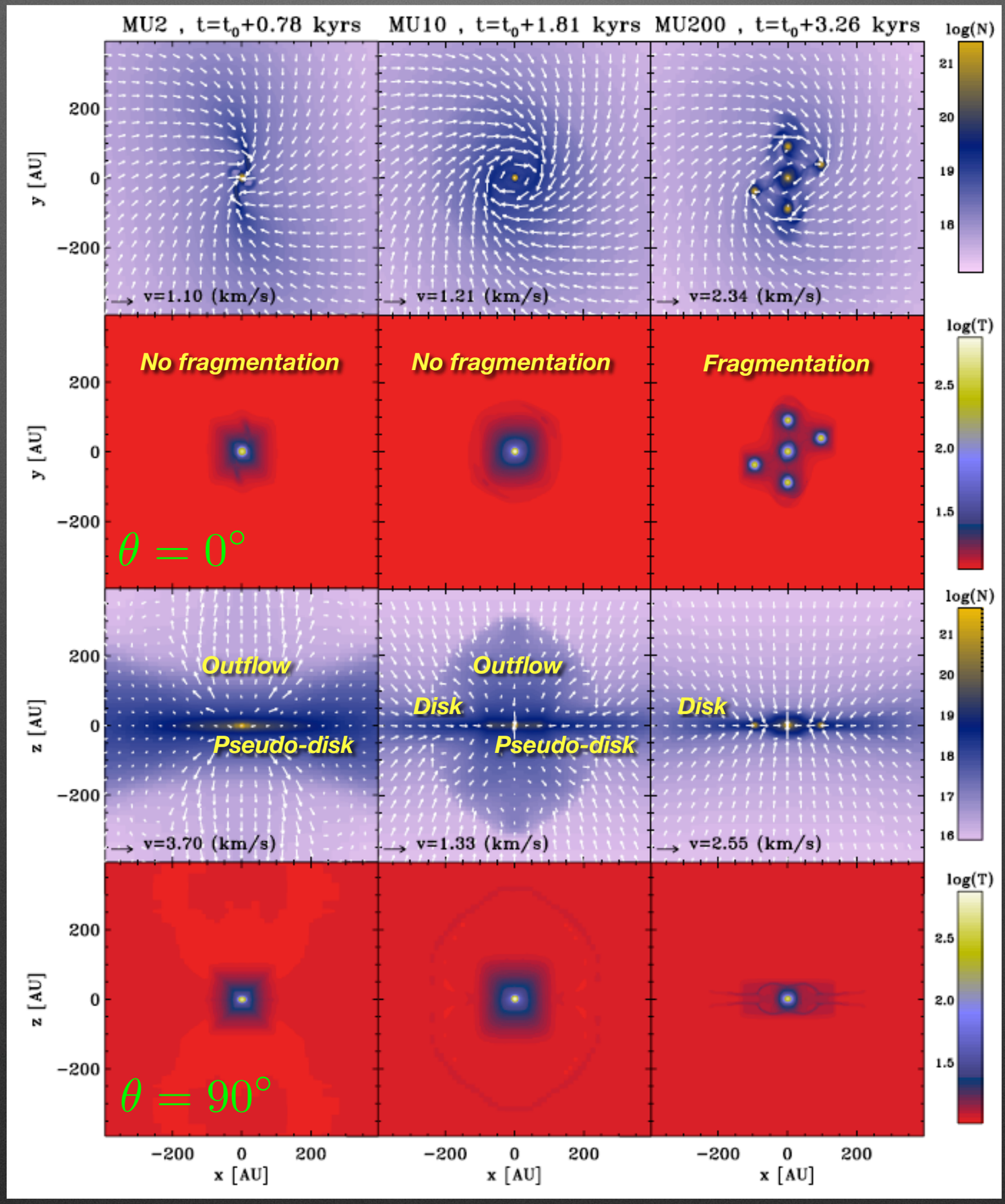
SPH simulation with 5,000,000 particles

Peretto, Hennebelle & André, 2007



Synthetic Position–Velocity Diagram



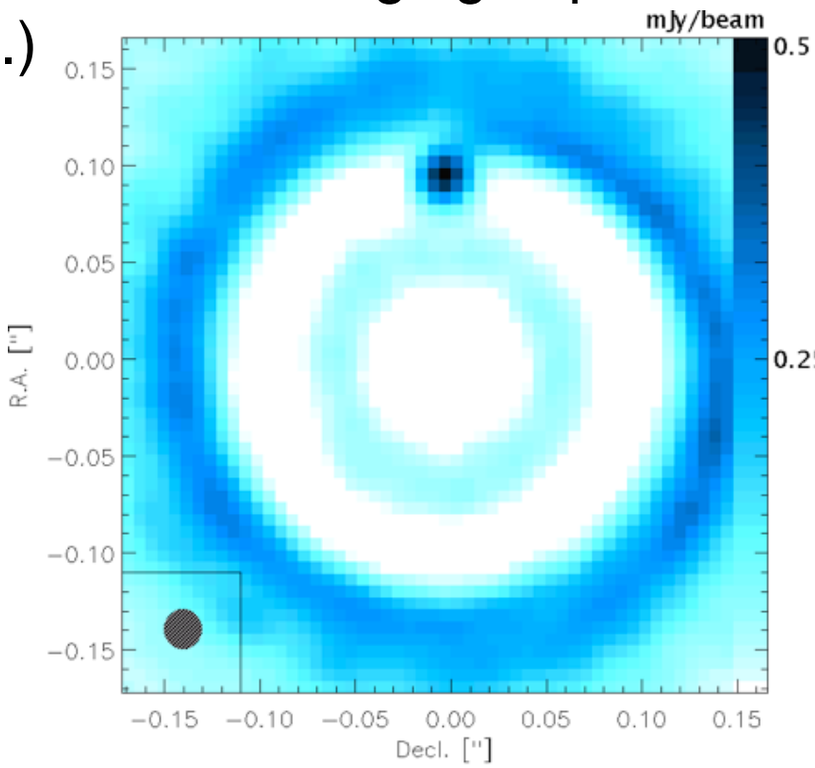

MU2 , t=t0+0.78 kyrs
MU10 , t=t0+1.81 kyrs
MU200 , t=t0+3.26 kyrs
log(N)
log(T)
y [AU]
z [AU]
x [AU]
v=1.10 (km/s)
v=1.21 (km/s)
v=2.34 (km/s)
No fragmentation
No fragmentation
Fragmentation
θ = 0°
Outflow
Pseudo-disk
Outflow
Disk
Pseudo-disk
Disk
v=3.70 (km/s)
v=1.33 (km/s)
v=2.55 (km/s)
θ = 90°

The ALMA Simulator in GILDAS

An **ALMA / ALMA Compact Array (ACA) / Single Dish** imaging simulator

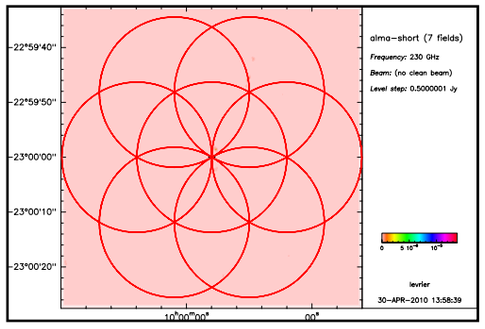
- Detailed description in ALMA memo 398 (Pety, Gueth, Guilloteau)
- Developed for studying the impact of ACA on wide-field imaging capabilities
- Scientific preparation of ALMA (e.g. Wolf et al.)
- Included in GILDAS' MAPPING software

http://www.iram.fr/IRAMFR/GILDAS/



1. Inputs

- Source position and size : mosaicing →
- Model brightness distribution
- Array configuration
- Frequency **(only continuum)**
- Type of observation (ALMA + ACA + Single Dish)



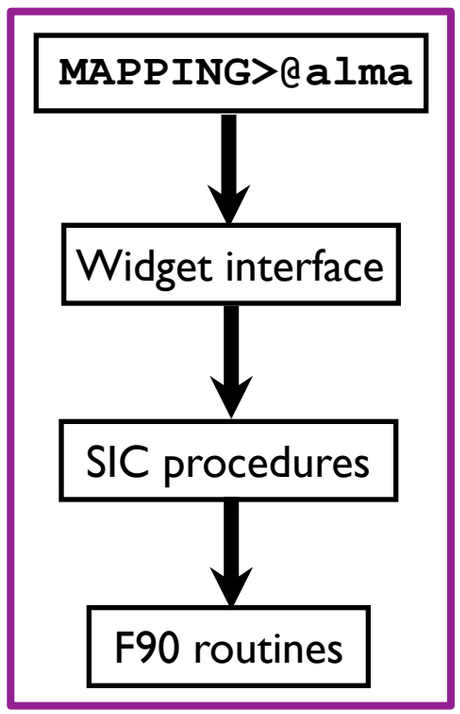
2. Visibilities

$$\text{Visibilities} = \text{Cover} \times \text{FT}[\text{Beam} \times \text{Model}]$$

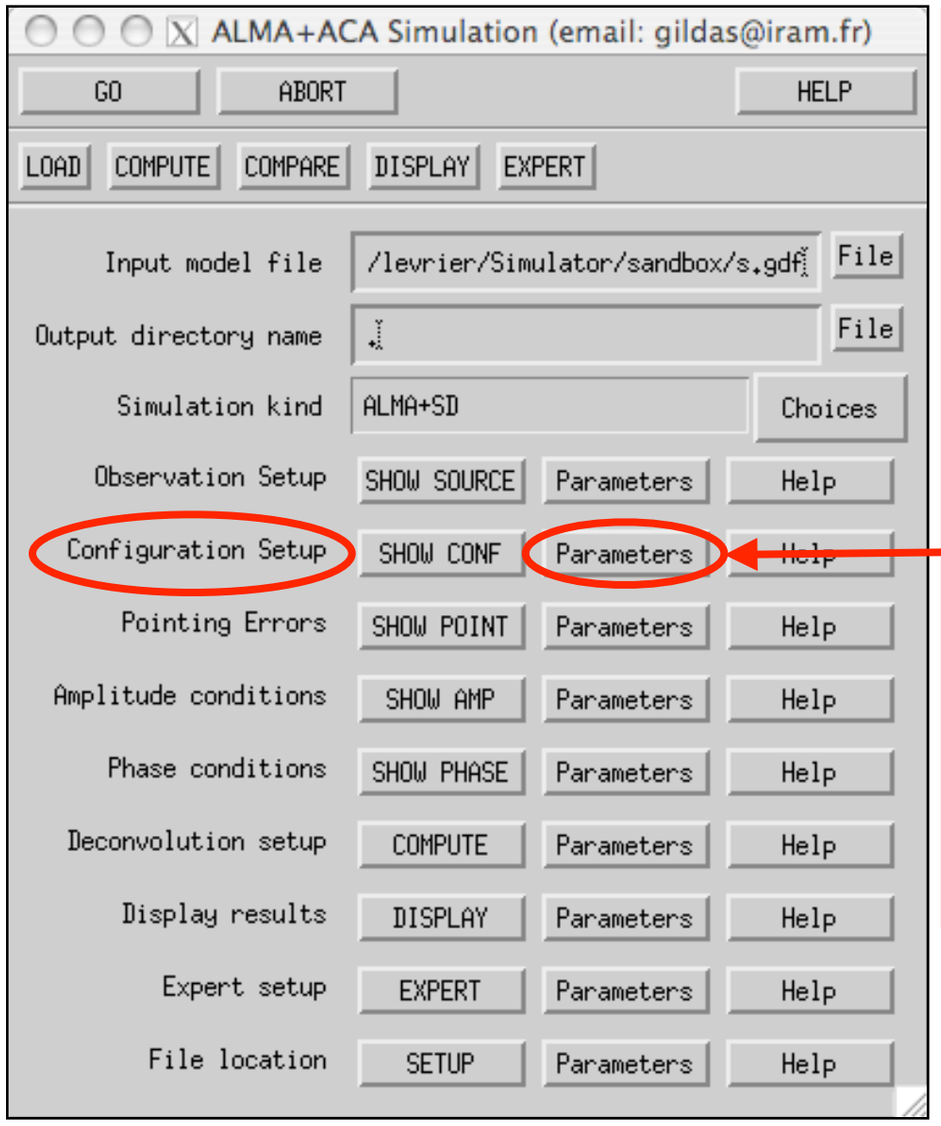
- Cover from source position, array configuration and time range
- Beam from antenna size
- Source-calibrator loop
- Possibility to add pointing errors, atmospheric phase noise, calibration errors

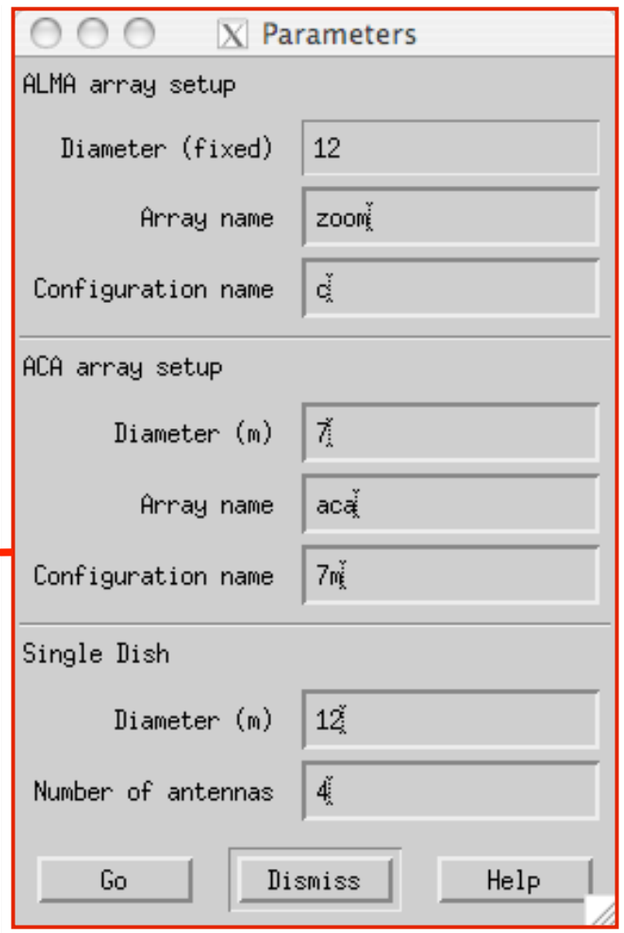
3. Imaging

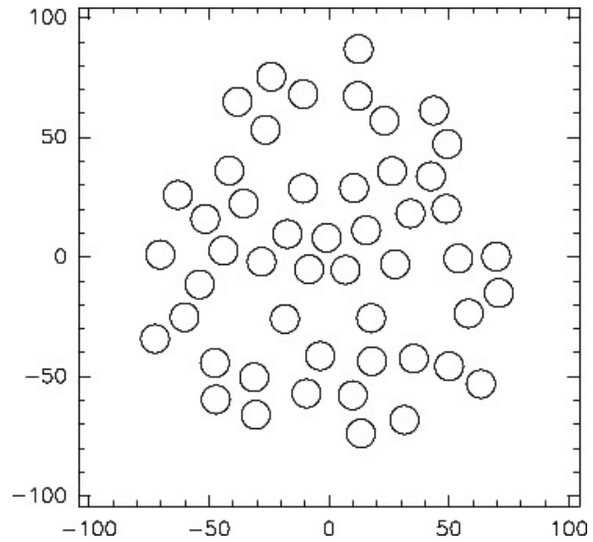
- Calibration (standard, fast switching, water vapor radiometry)
- Deconvolution (Standard CLEAN based methods)
- Input and output comparison



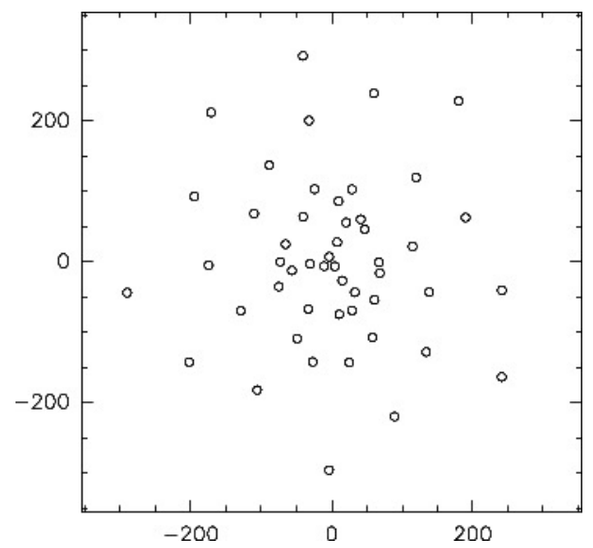
Up-to-date ALMA configurations



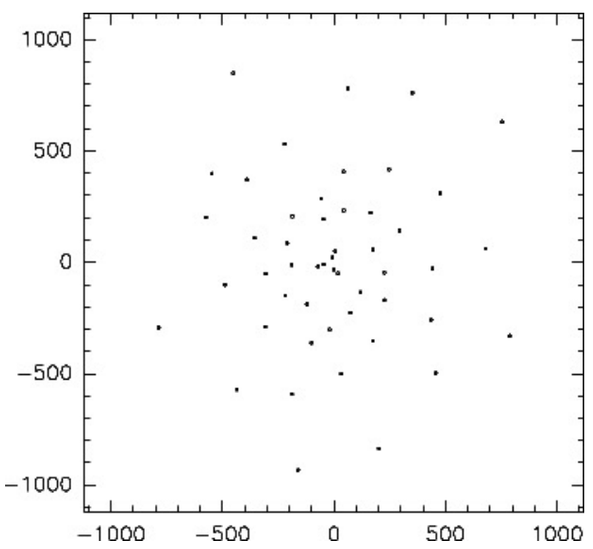




#1



#8

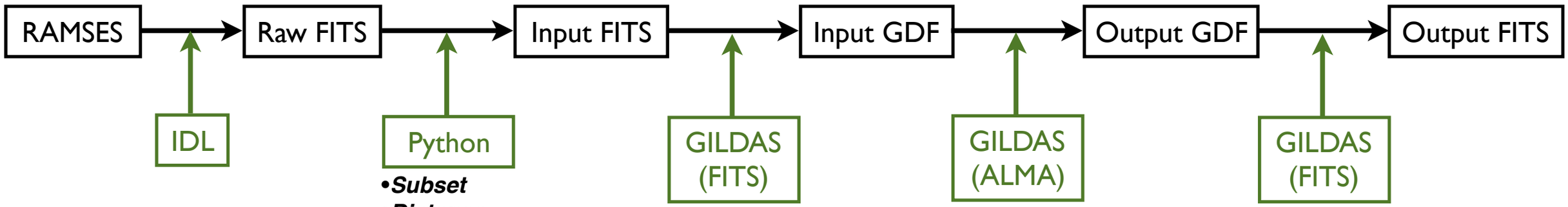


#15

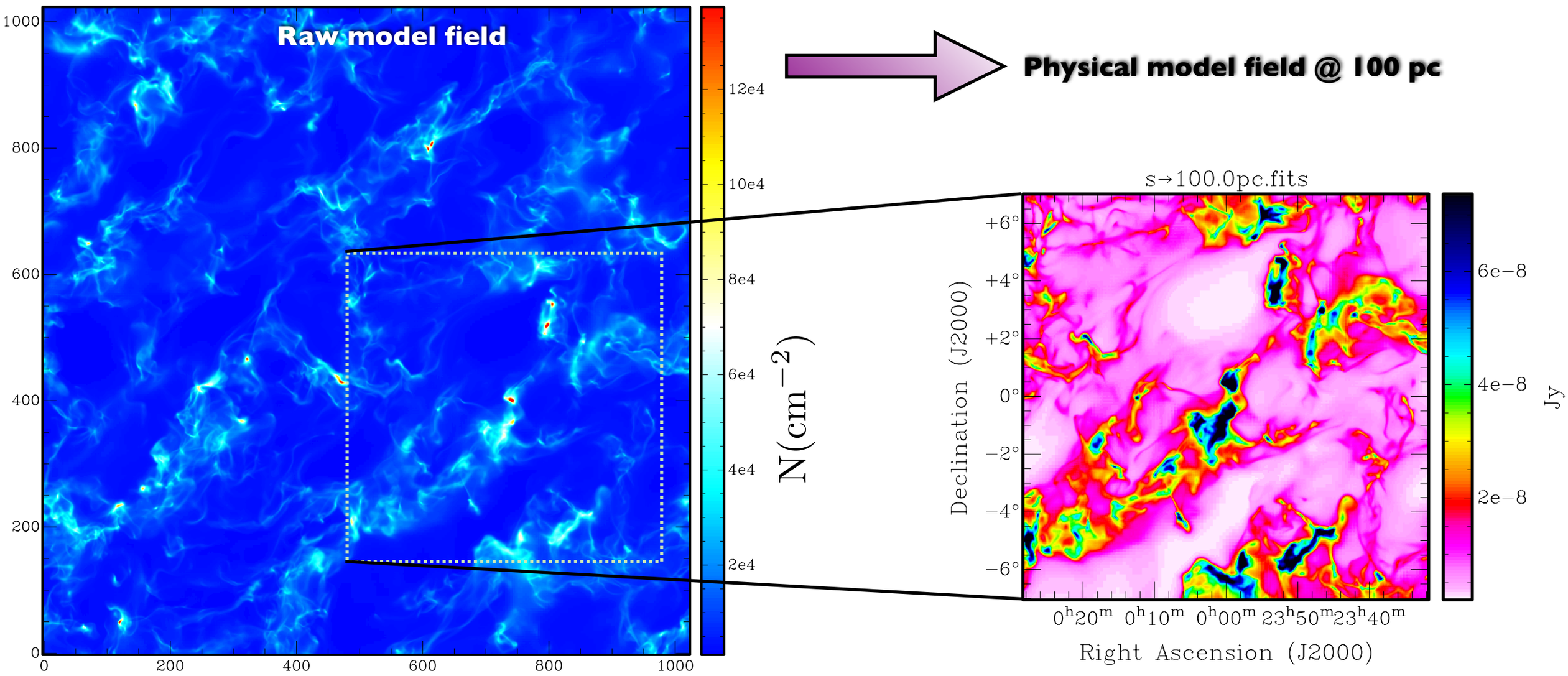
- *28 configurations*
- *From 90 m to 9.5 km radius*
- *CASA to GILDAS format conversion*

Thanks to J. Pety, A. Wooten, I. Heywood, K.-I. Morita

ALMA simulator on MHD simulations



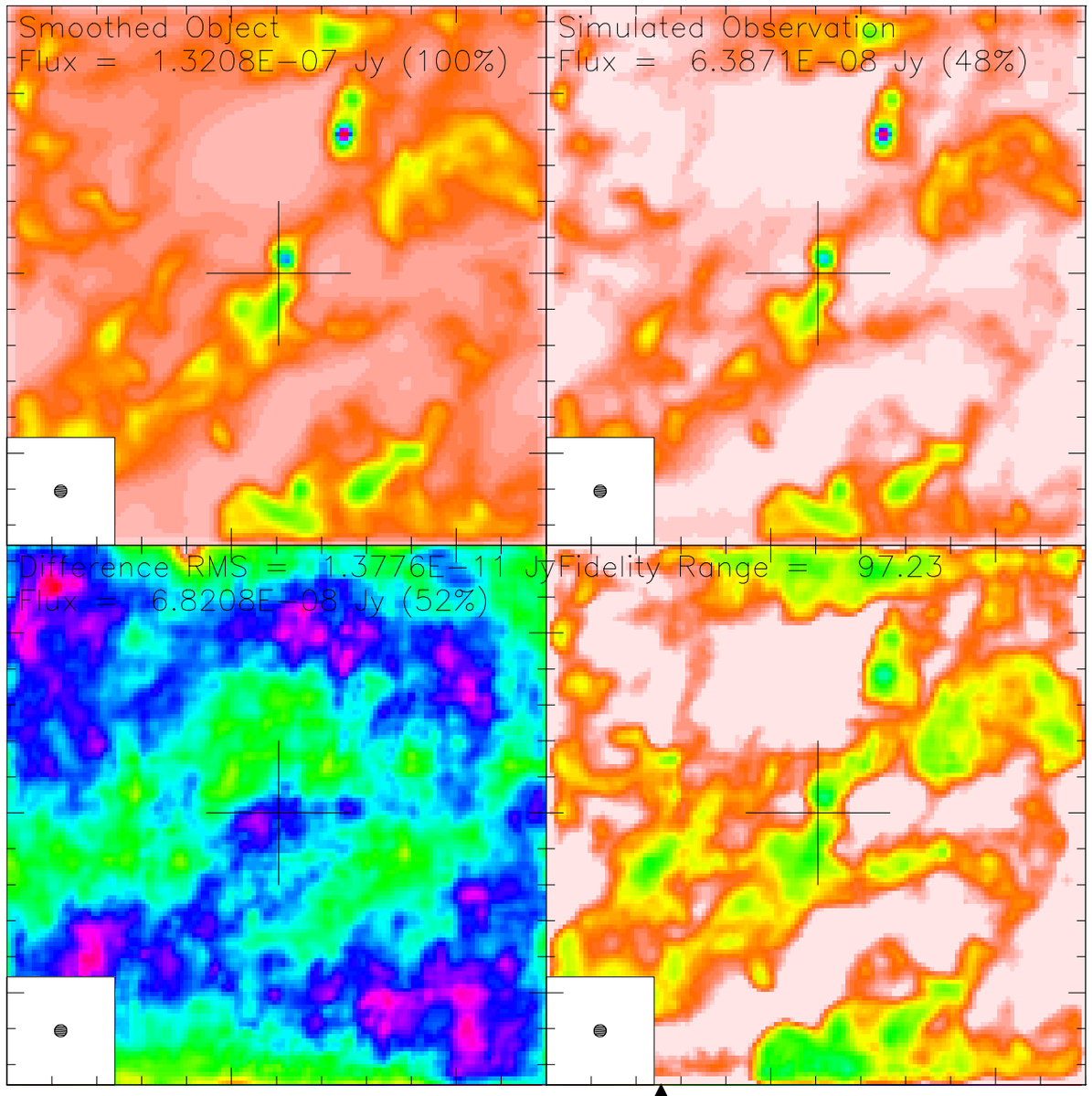
- ***Subset***
- ***Distance***
- ***Brightness temperature***
- ***Sky position***



Simulated observations of large-scale flows

ALMA only **Flux recovered : 48%**

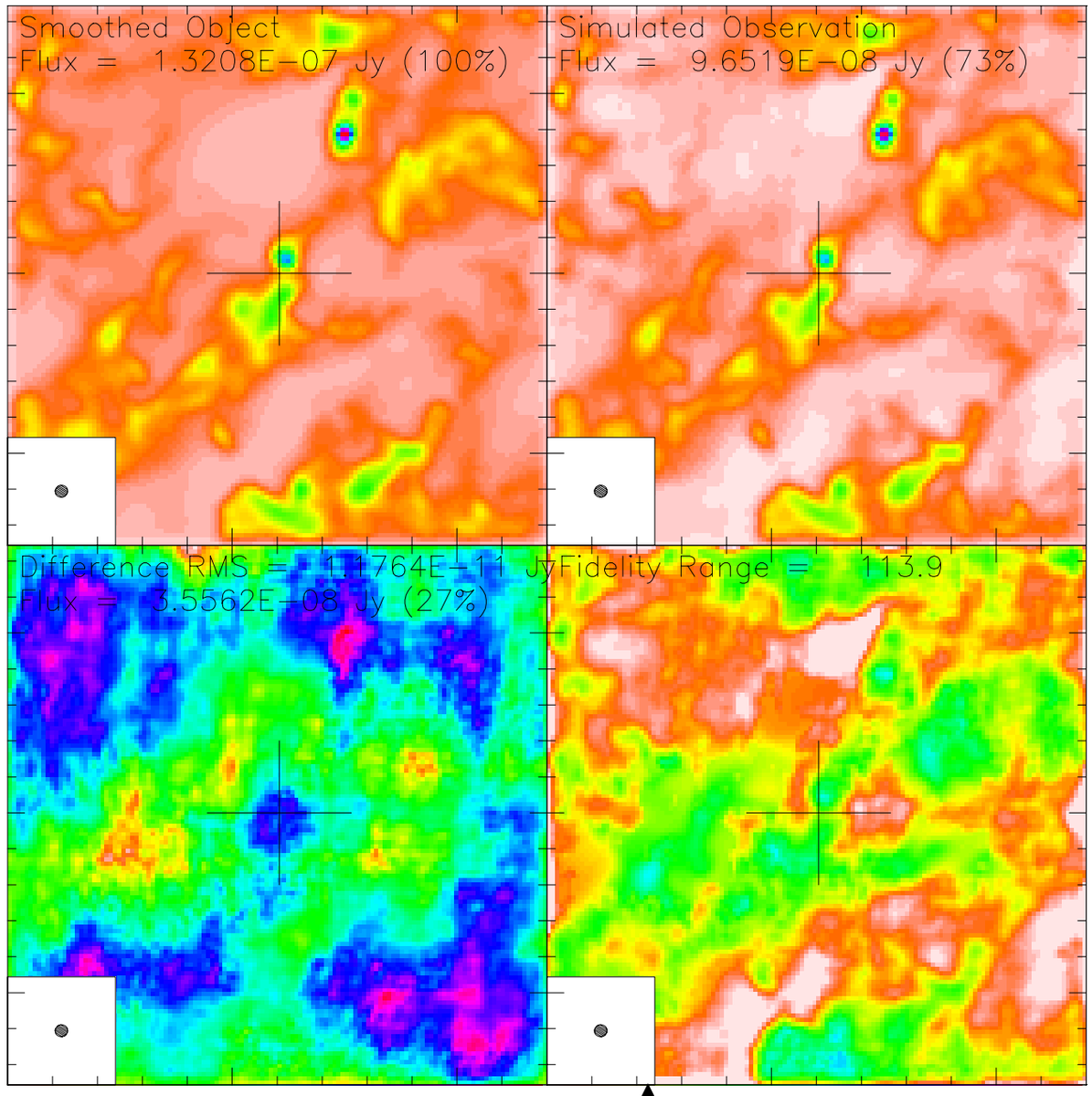
Smoothed input *Simulated observation*



Difference *Fidelity*

ALMA + Single Dish **Flux recovered : 73%**

Smoothed input *Simulated observation*



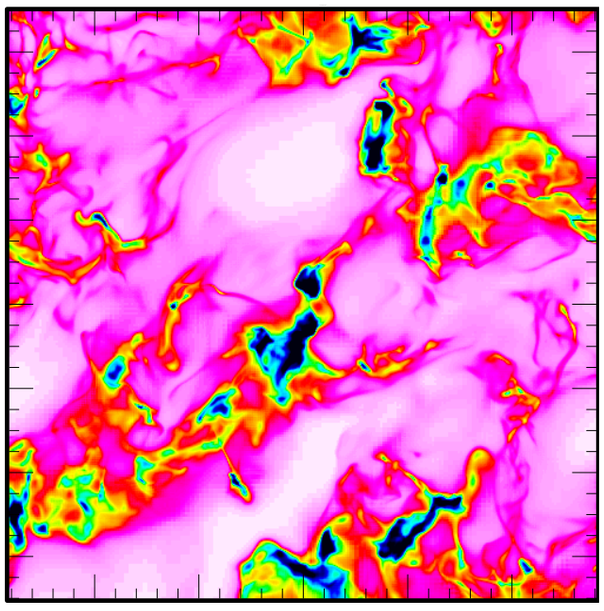
Difference *Fidelity*

Fidelity image = input model / difference

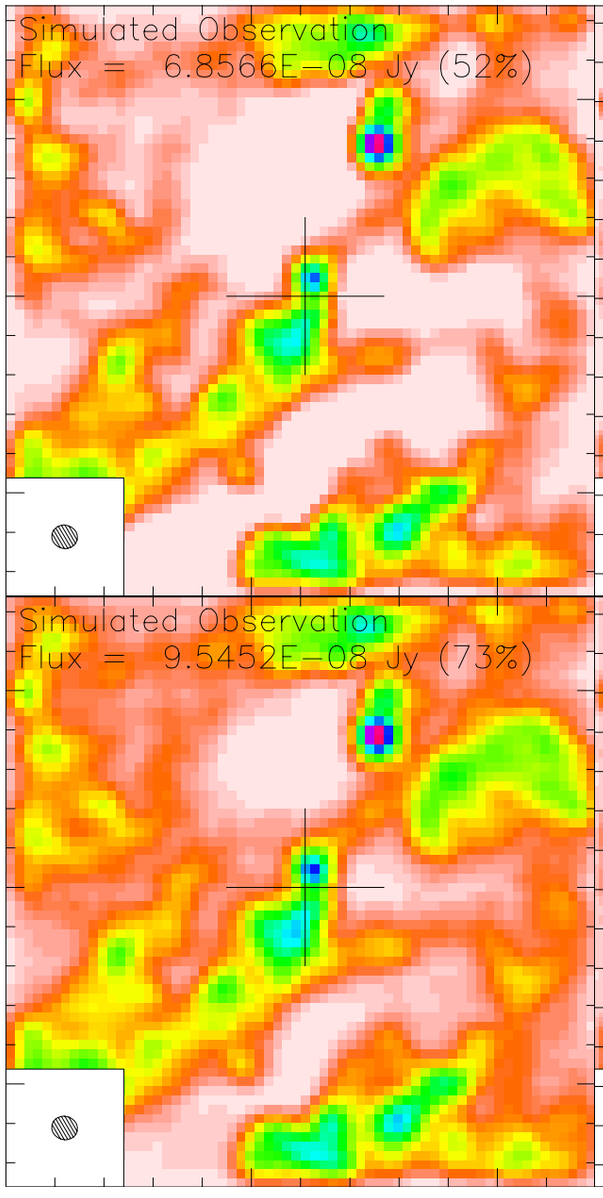
- **Inverse of relative error**
- **In practice, lowest values of difference are truncated**

Simulations for different configurations

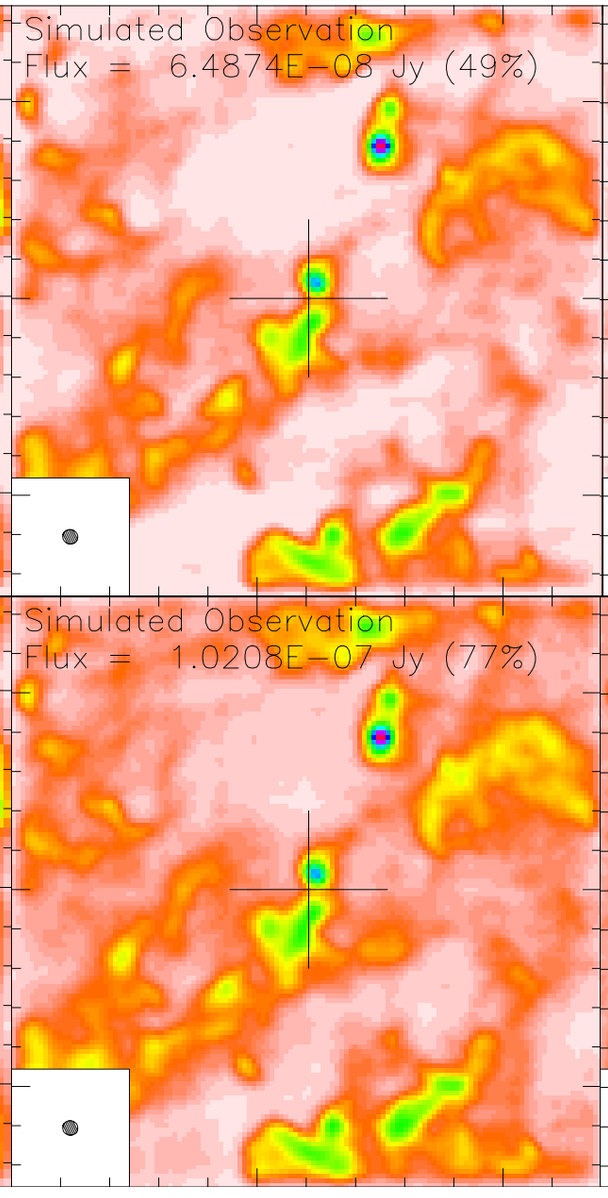
Original field



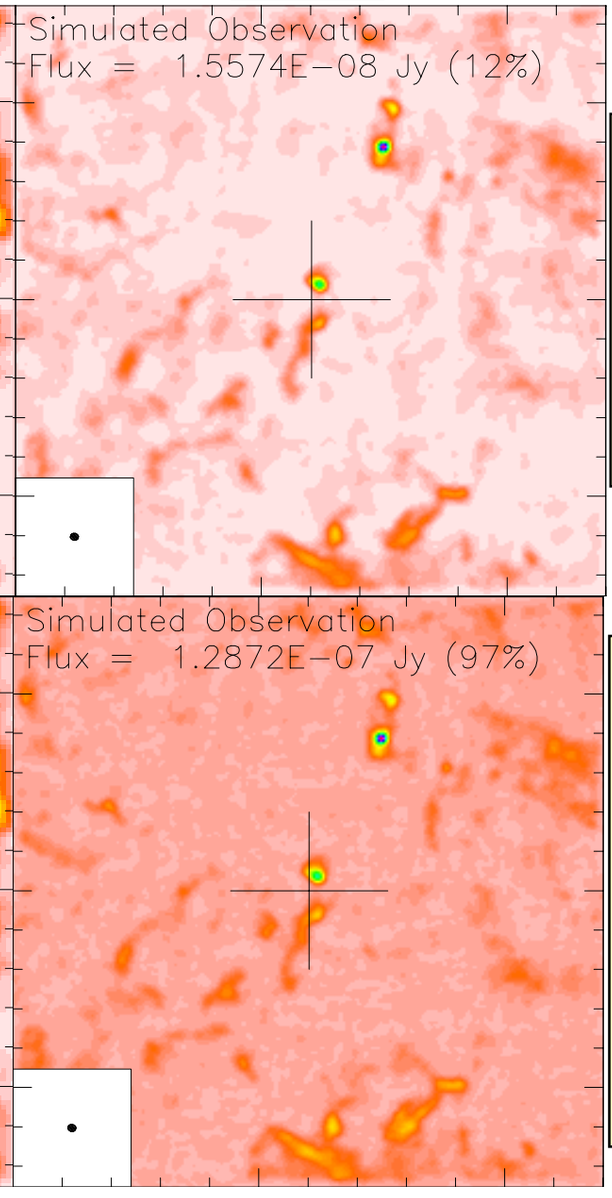
#8



#11



#15

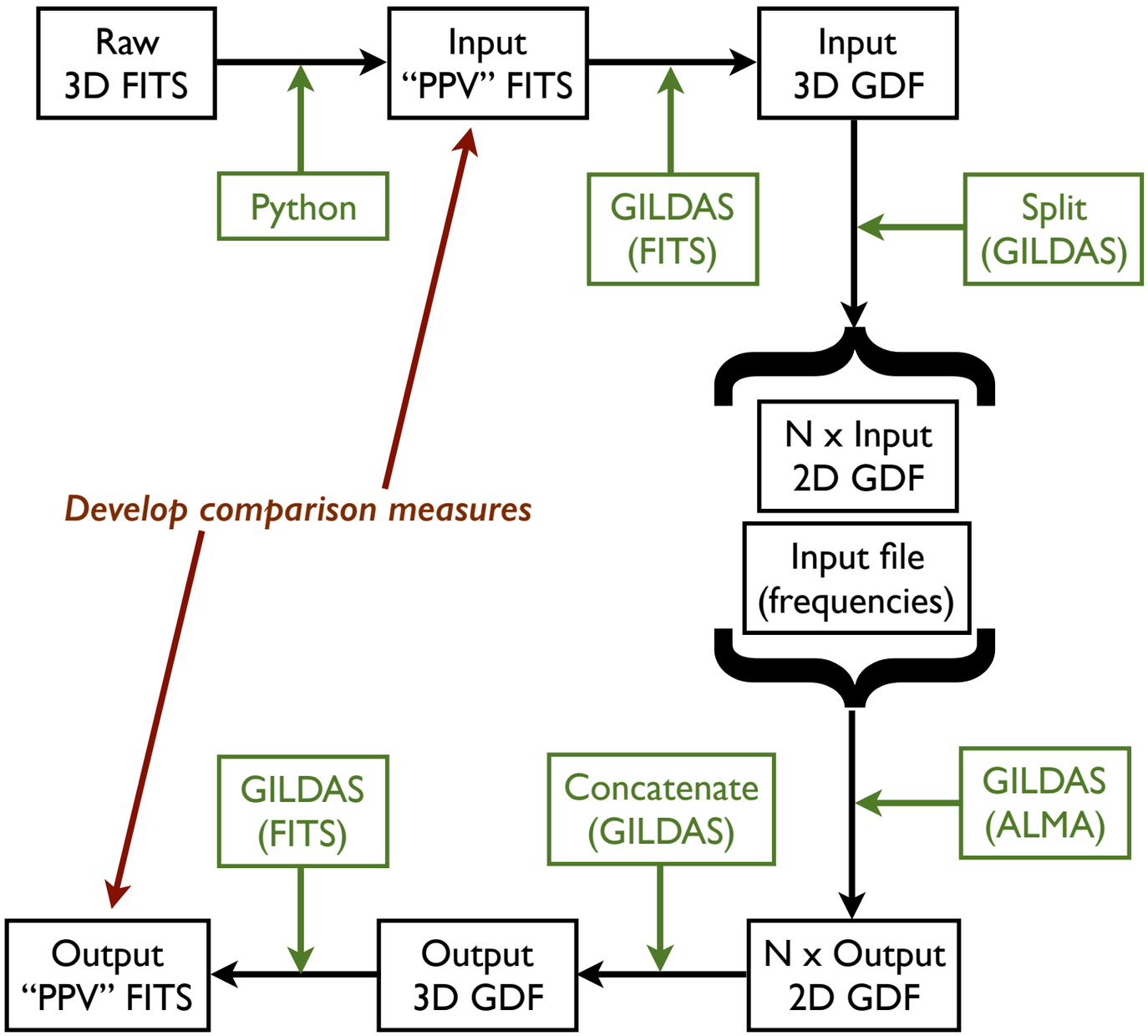


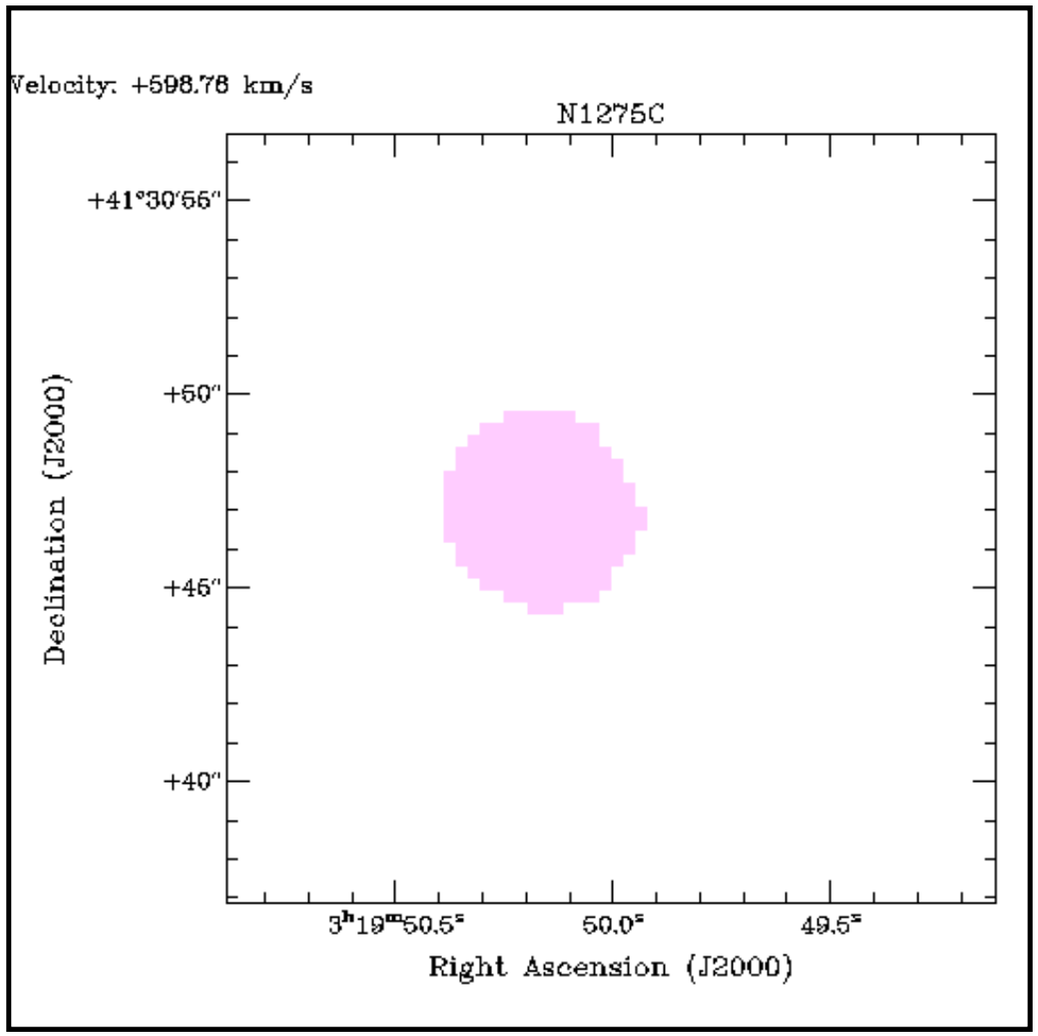
ALMA only

ALMA + Single Dish

- Spatial frequency filtering
- Flux loss
- Importance of single-dish measurements

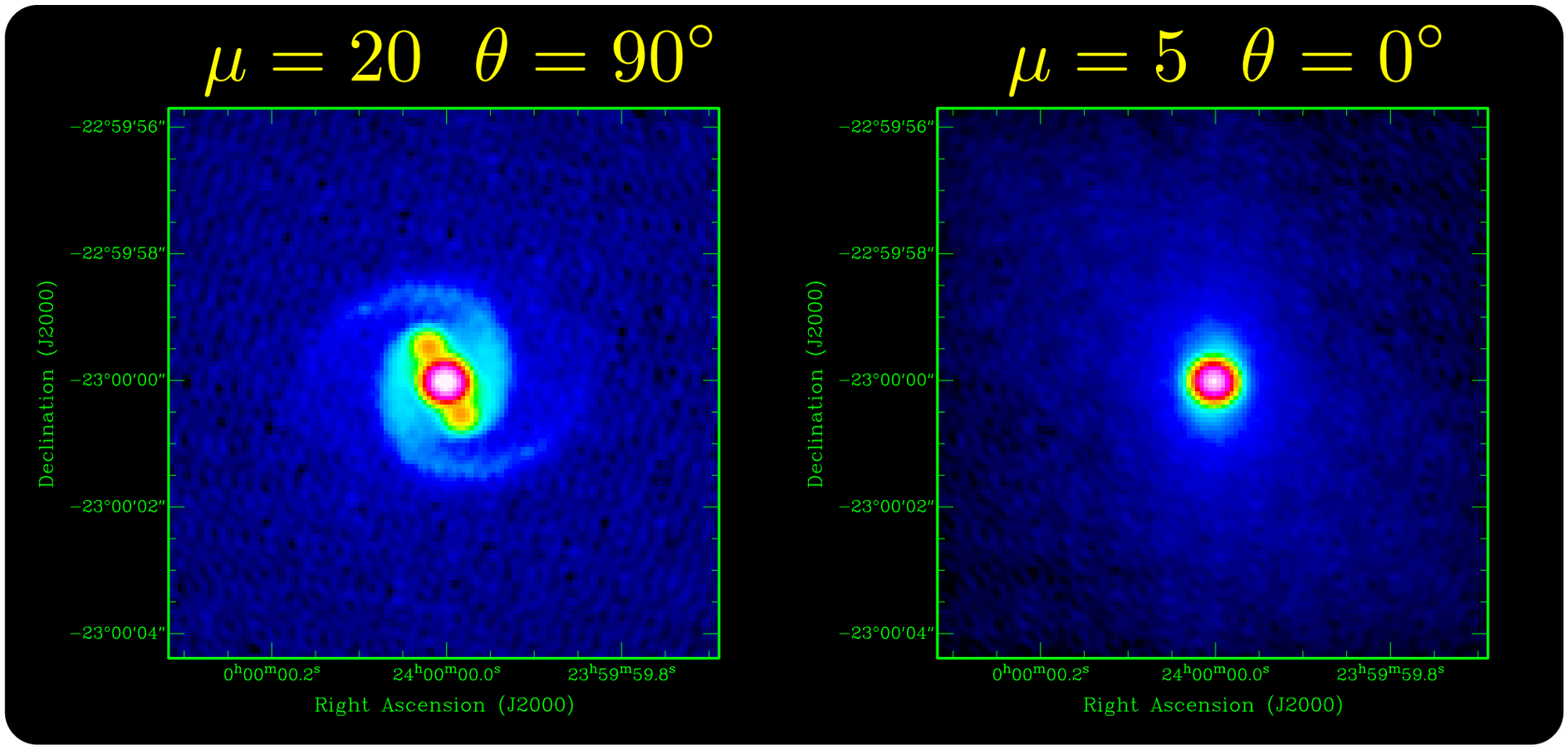
“Line” mapping using batch mode

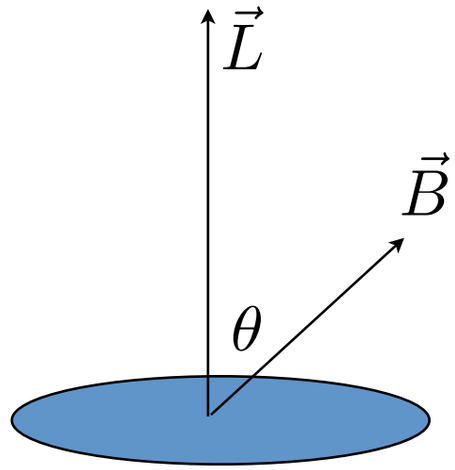




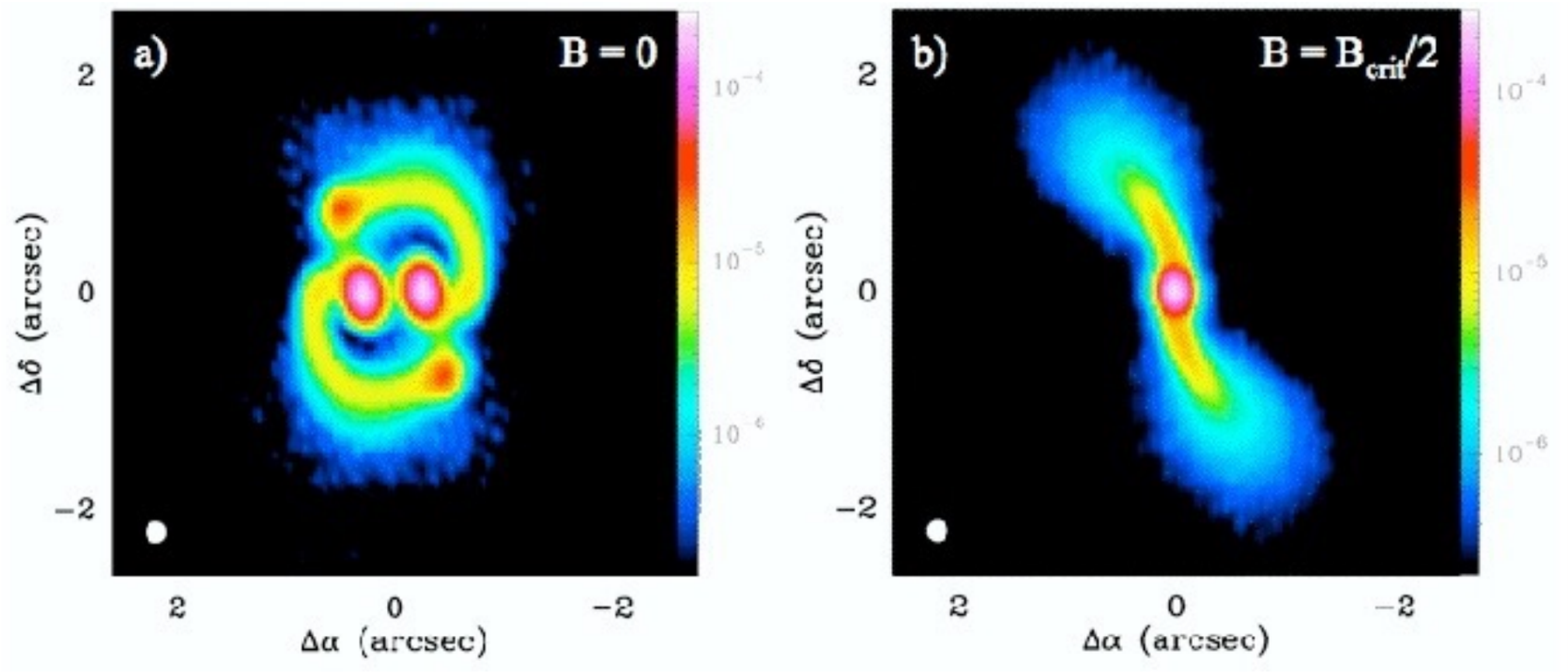
Simulated ALMA observations of collapsing cores

ALMA band 7 (.....) images for configuration #10



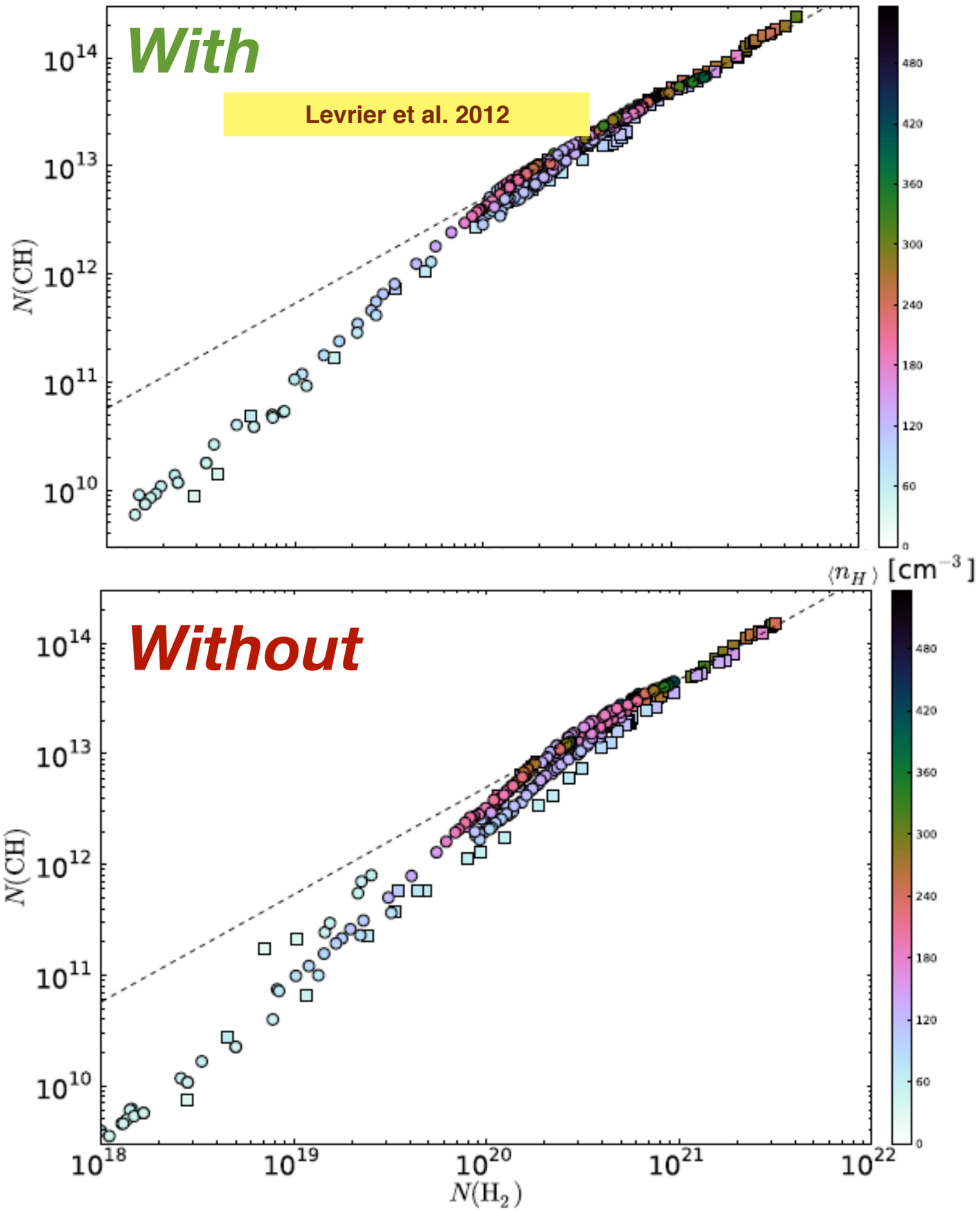


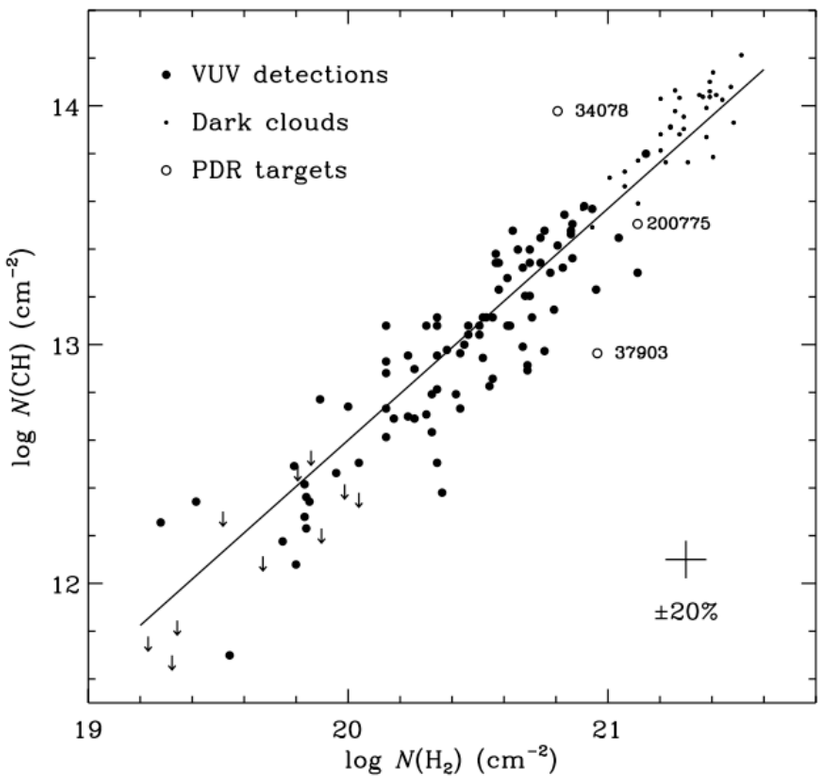
$$\mu = \frac{(M/\Phi)}{(M/\Phi)_{\rm crit}}$$



André, Hennebelle, Peretto 2008

Density fluctuations vs. Uniform density : CH





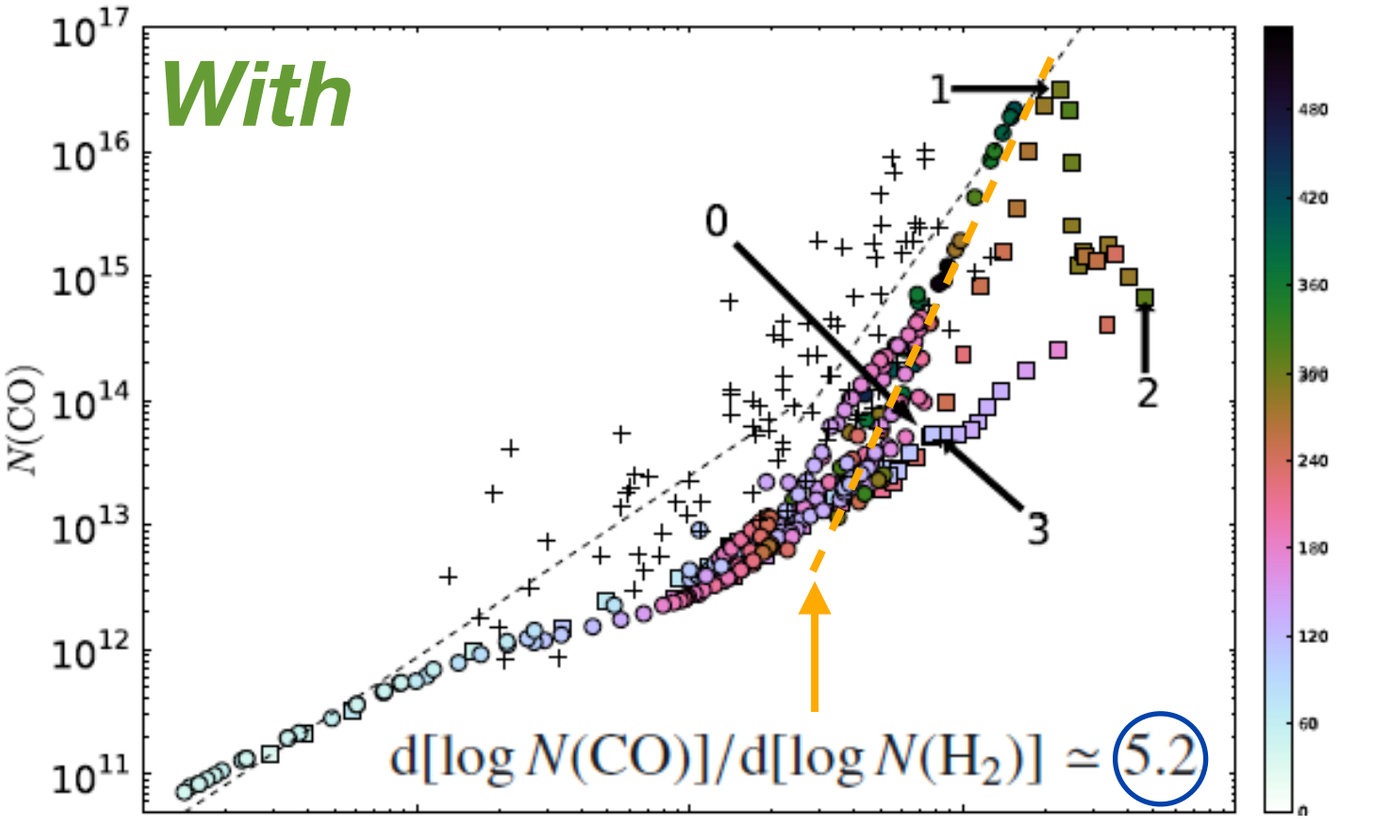
Observational fit

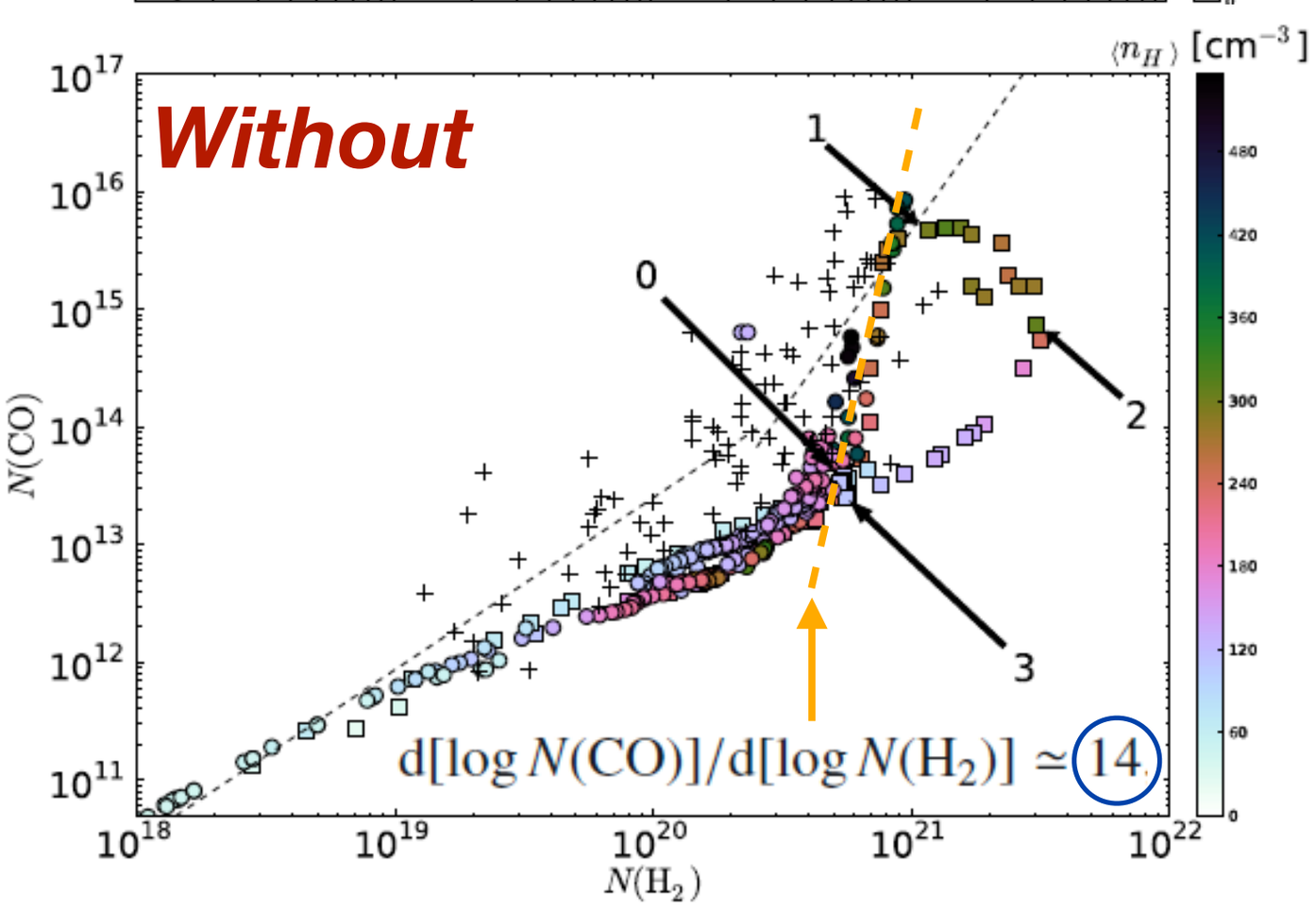
$$\mathrm{d}\left[\log N\left(\mathrm{CH}\right)\right]/\mathrm{d}\left[\log N\left(\mathrm{H_2}\right)\right] \simeq 1.09 \pm 0.19$$

Sheffer et al. 2008

- Maximum column densities are about twice as low in the uniform models
- CO vs CH column densities correlation agrees better with observations

Density fluctuations vs. Uniform density : CO





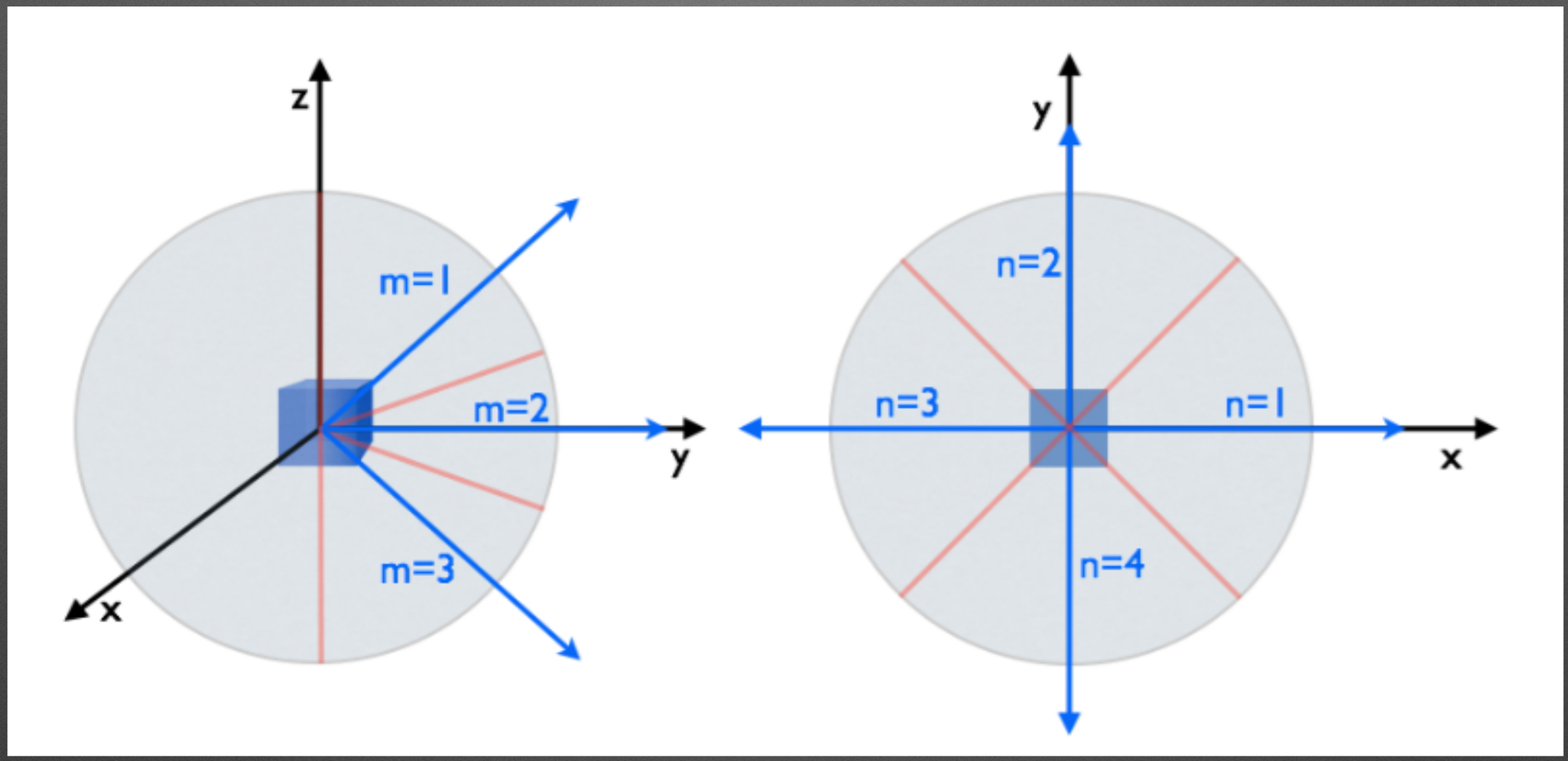
Observational fit

$$d[\log N(CO)]/d[\log N(H_2)] \simeq 3.07 \pm 0.73$$

Sheffer et al. 2008

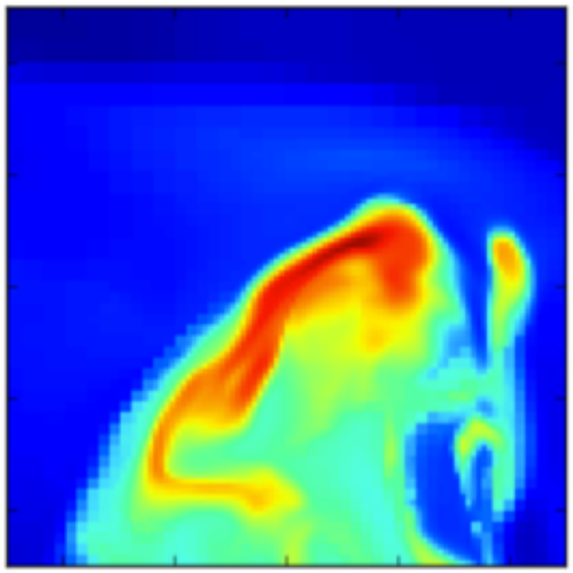
- Maximum column densities are about 3 times as low in the uniform models
- CO vs H_2 column densities correlate better

The influence of screening on ISM structures

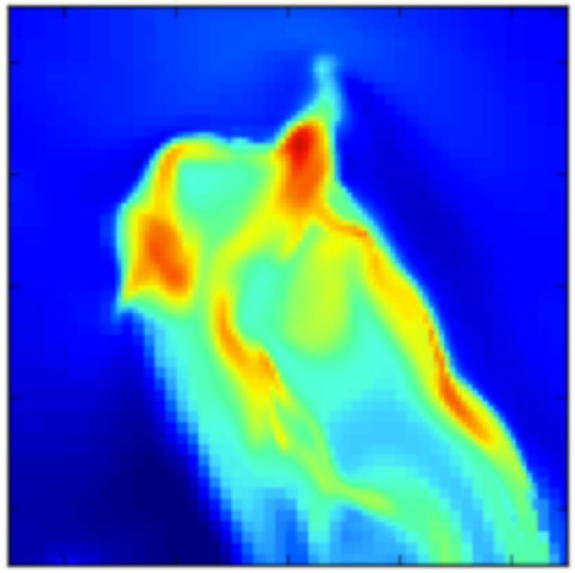


Without screening

With screening



Valdivia & Hennebelle (2014)



Turbulence in the interstellar medium ?

THE EVOLUTION OF GALAXIES AND STARS

C. F. VON WEIZSÄCKER
Max Planck Institut, Göttingen
Received May 17, 1951

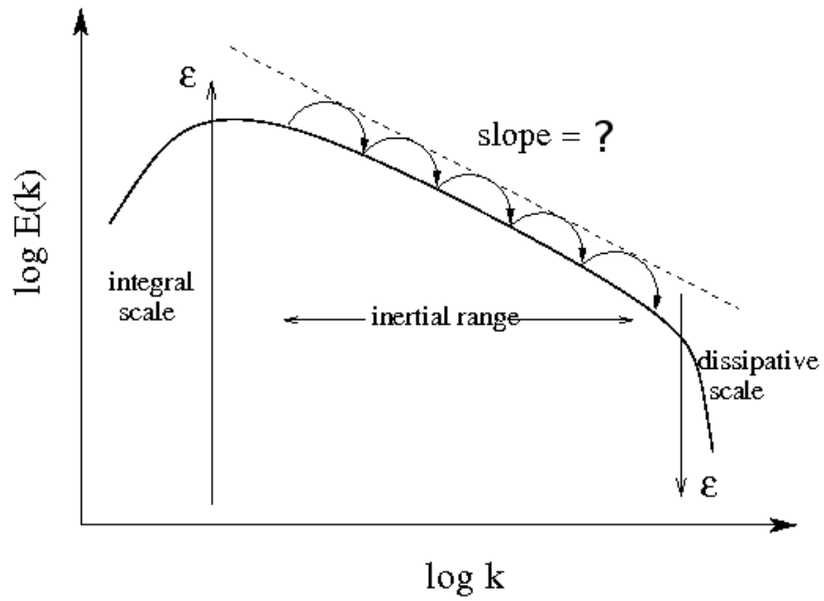
ABSTRACT

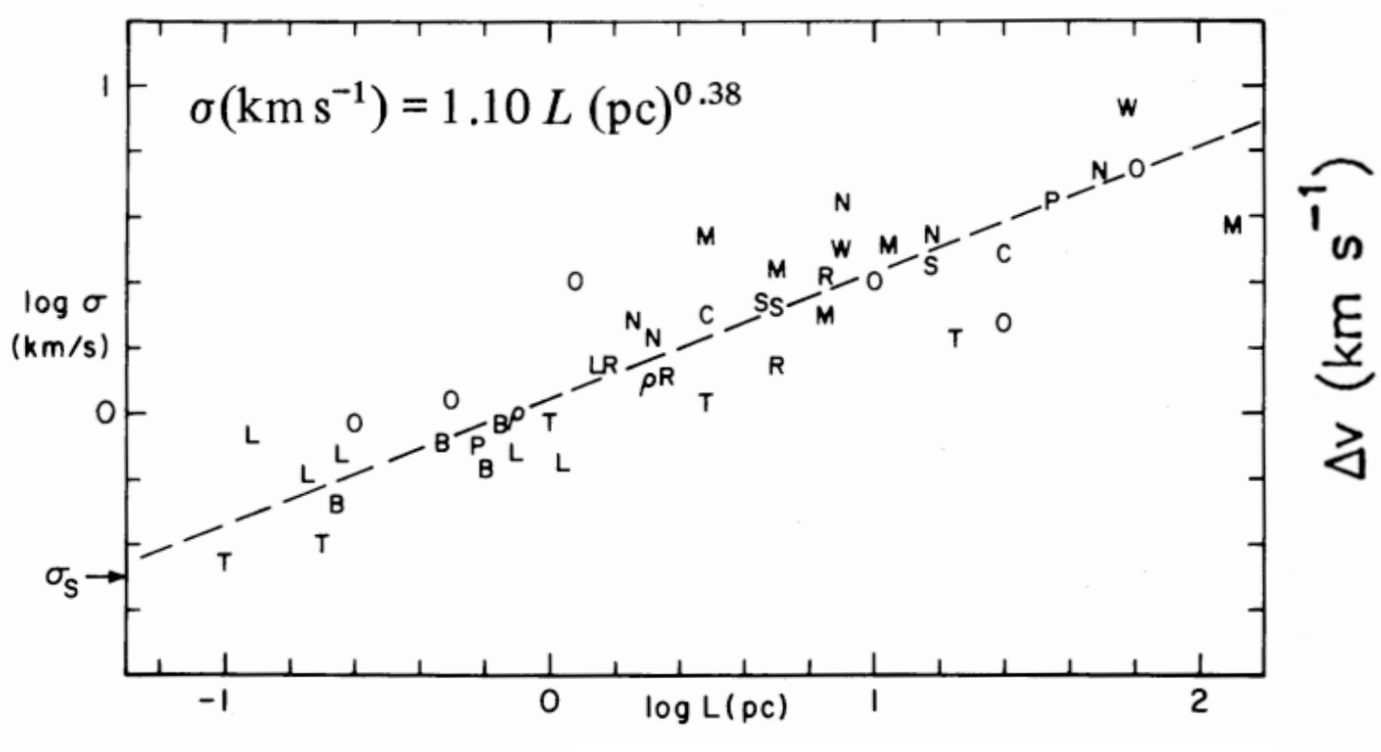
I. Aims of the theory.—A hydrodynamical scheme of evolution is proposed, confined to events after the time when the average density in the universe was comparable to the density inside a galaxy at our time.

II. Hydrodynamical conditions.—Gas in cosmic space is moving according to hydrodynamics, mostly in a turbulent and compressible manner. Dust is carried with the gas, probably by magnetic coupling. Star systems cannot be described hydrodynamically and hence do not show turbulence and supersonic compressibility.

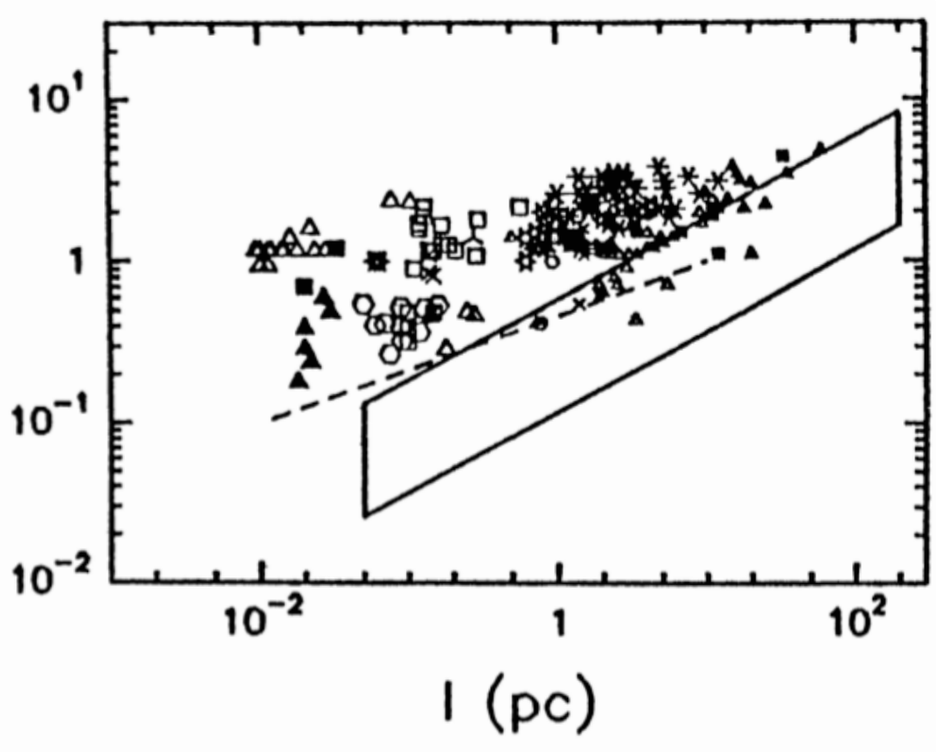
III. The spectral law of incompressible turbulence.—The relative velocity of two points at a distance l is proportional to $l^{1/3}$. This is deduced from the picture of a hierarchy of eddies.

IV. Compressibility and interstellar clouds.—A hierarchy of clouds is considered.





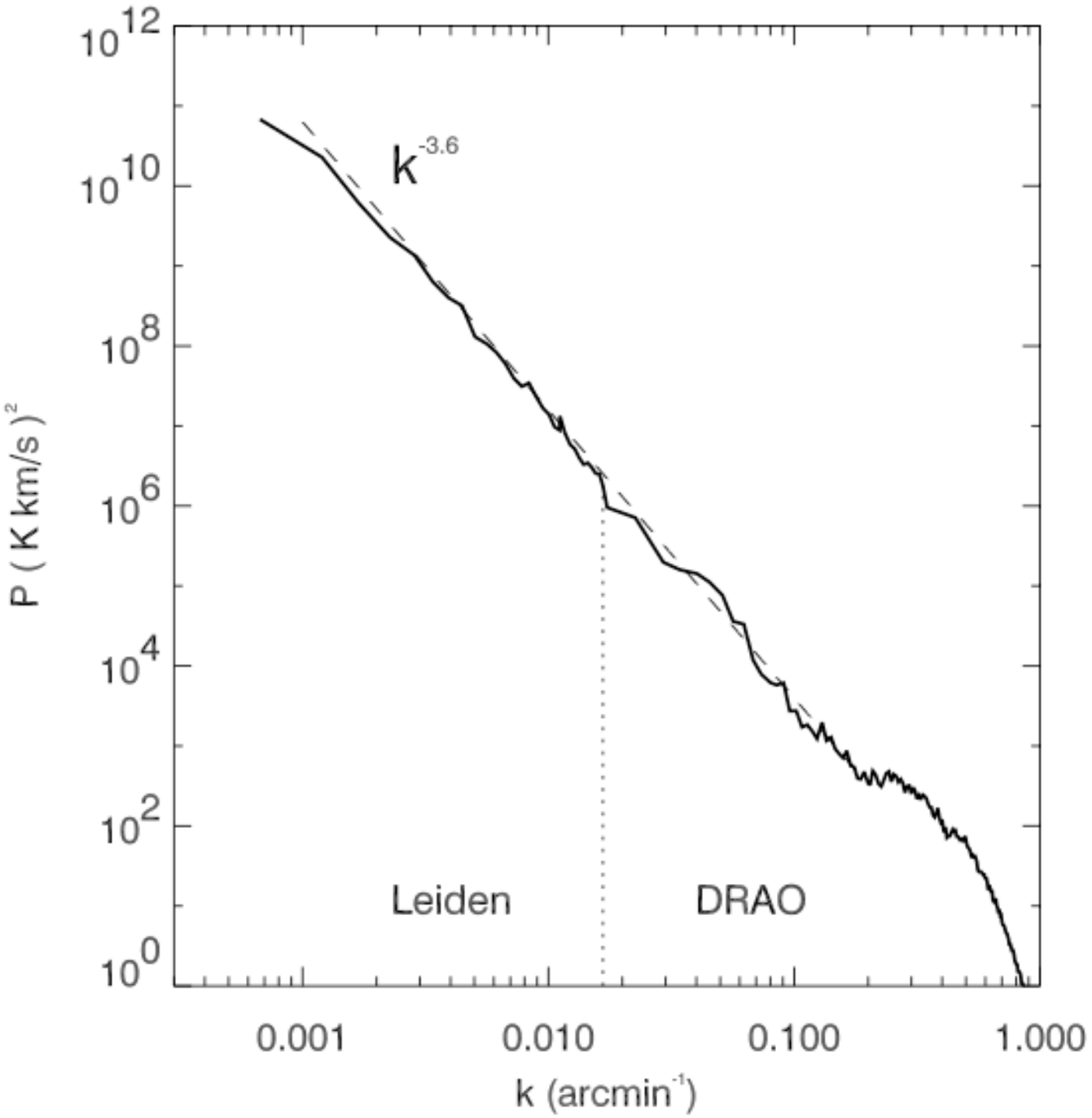
Larson, 1981



Falgarone, 1997

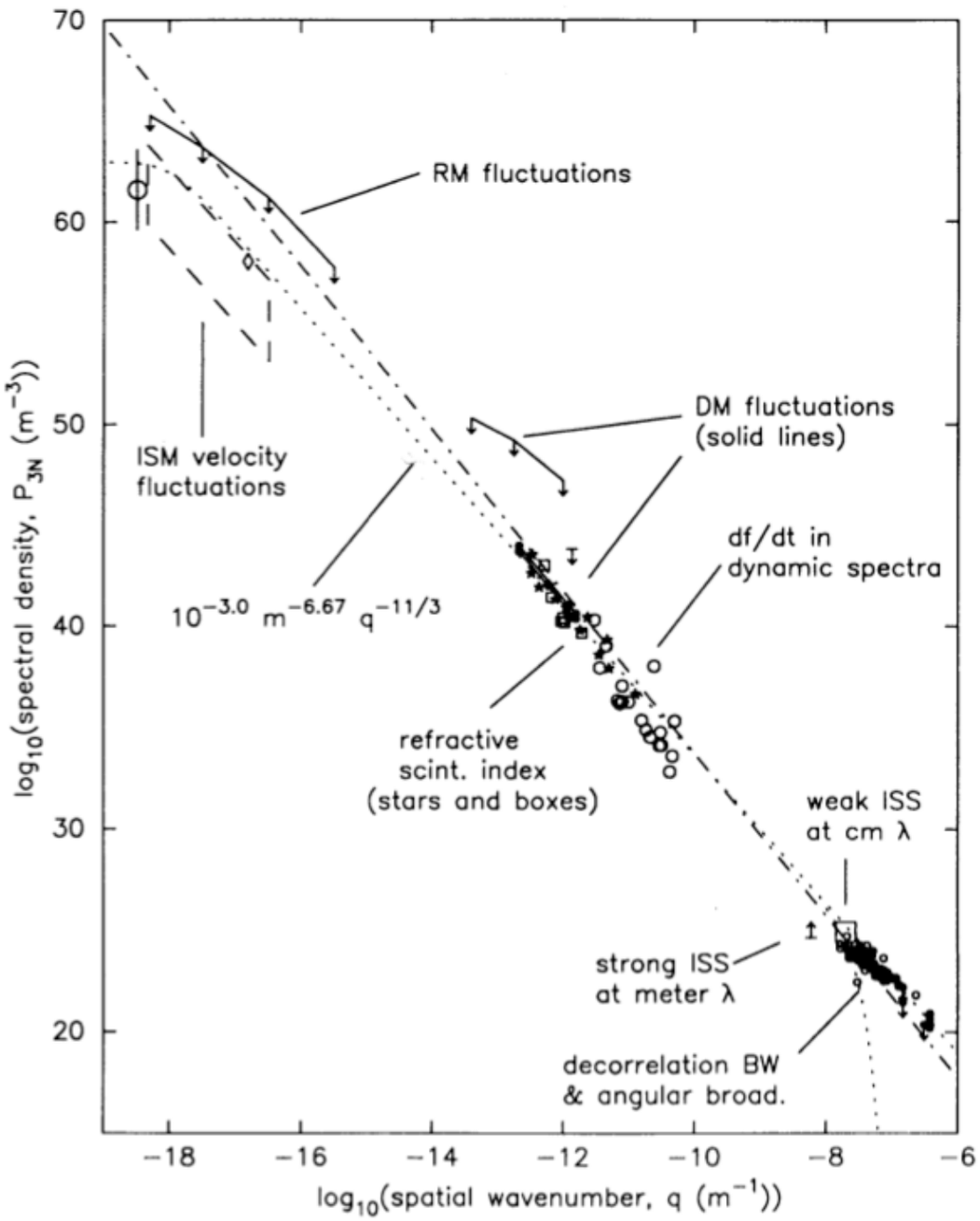
Power spectra in various phases

HI gas in Ursa Major



Miville-Deschênes et al., 2003

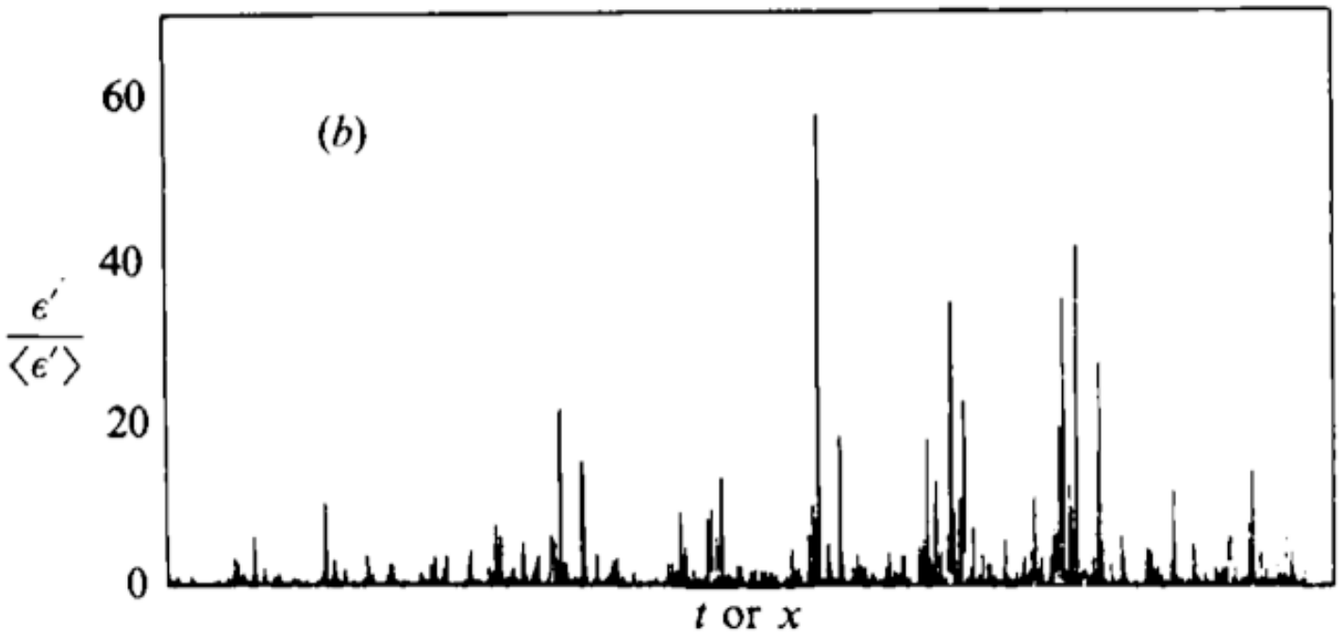
Electron density in local ISM



Armstrong et al., 1995

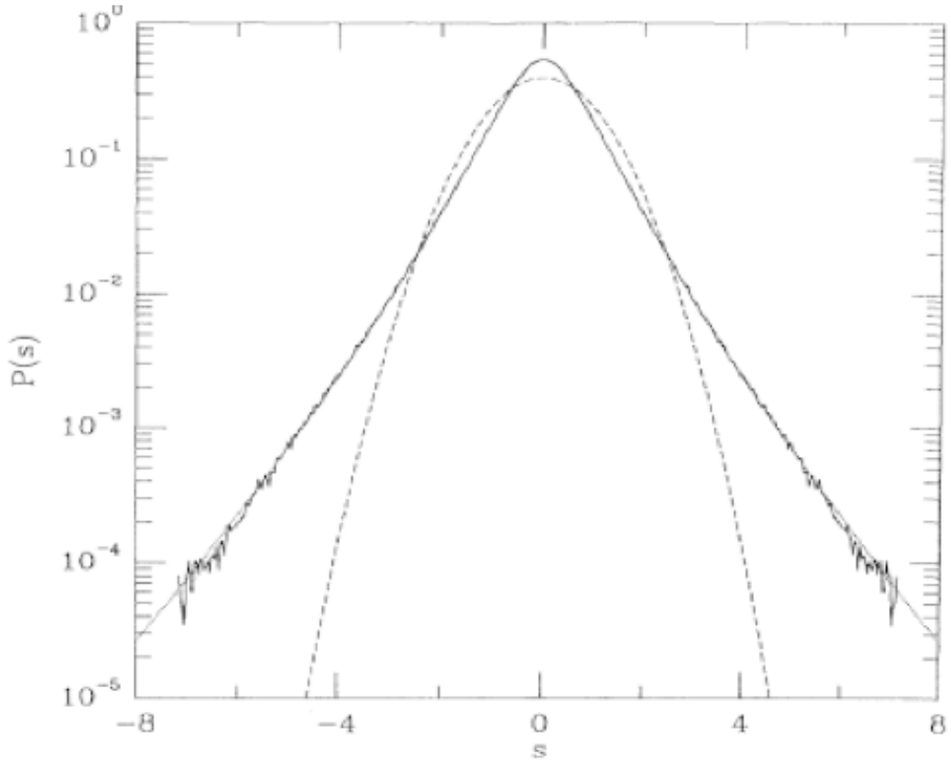
Intermittent dissipation of turbulence

Temporal series of the dissipation rate



Meneveau & Sreenivasan, 1991

Experimental PDF of velocity increments

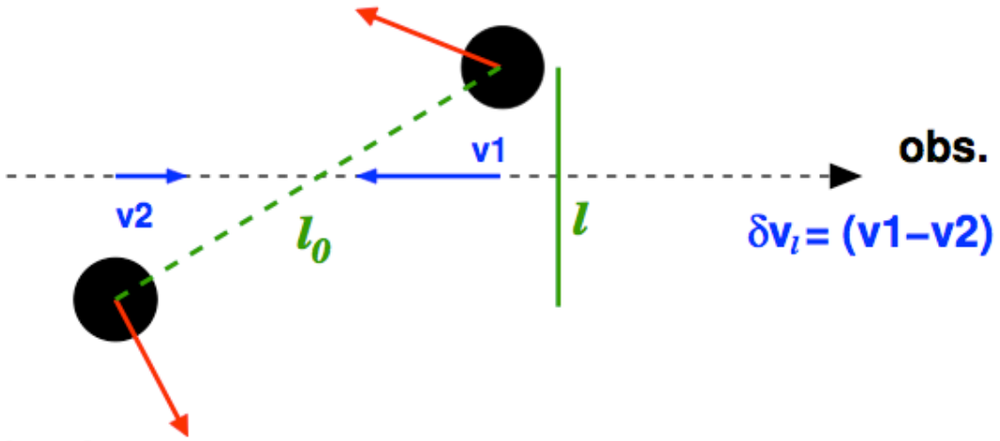


She 1991, Belin et al., 1996

Viscous dissipation rate $\left\langle \epsilon_d \right\rangle = \nu \left| \nabla \times \boldsymbol{v} \right|^2$

Problem : we cannot trace the vorticity ! $v_z(x, y)$

Centroid Velocity Increments

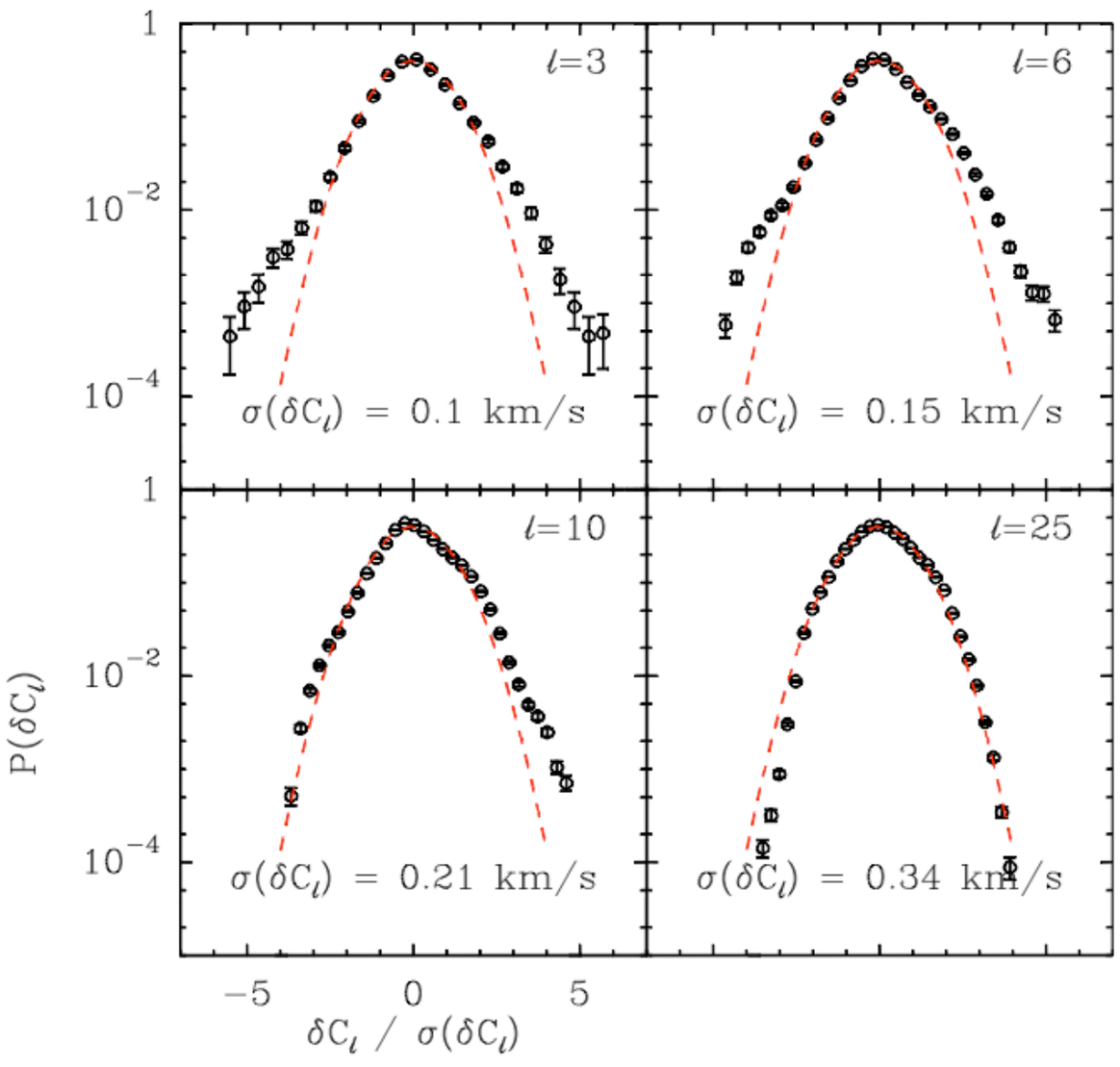


Line centroid velocity:

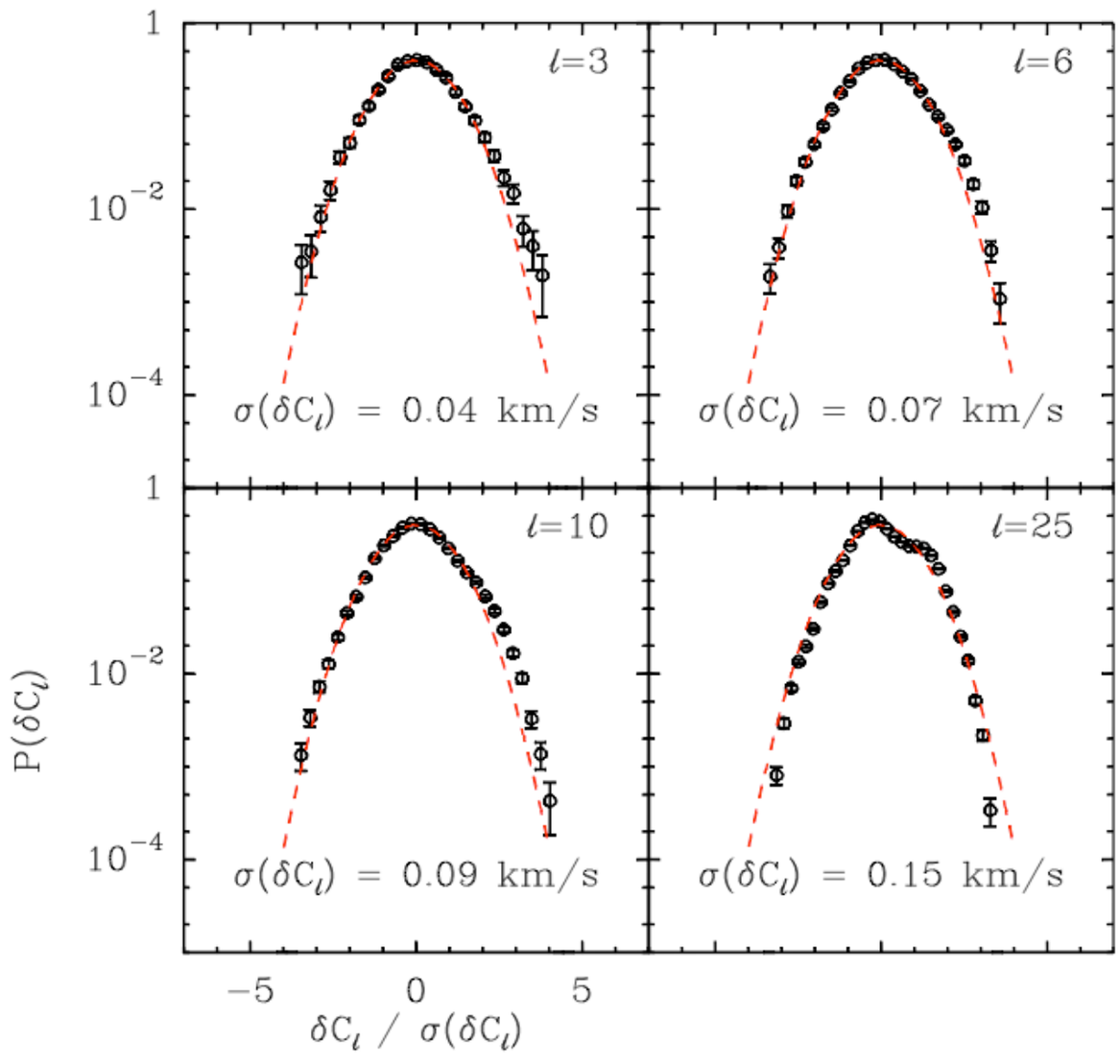
$$C(\mathbf{r}) = \int T(\mathbf{r}, v_x) v_x dv_x / \int T(\mathbf{r}, v_x) dv_x$$

Miesch & Scalo 1999, Pety & Falgarone 2003, Levrier 2004

Polaris



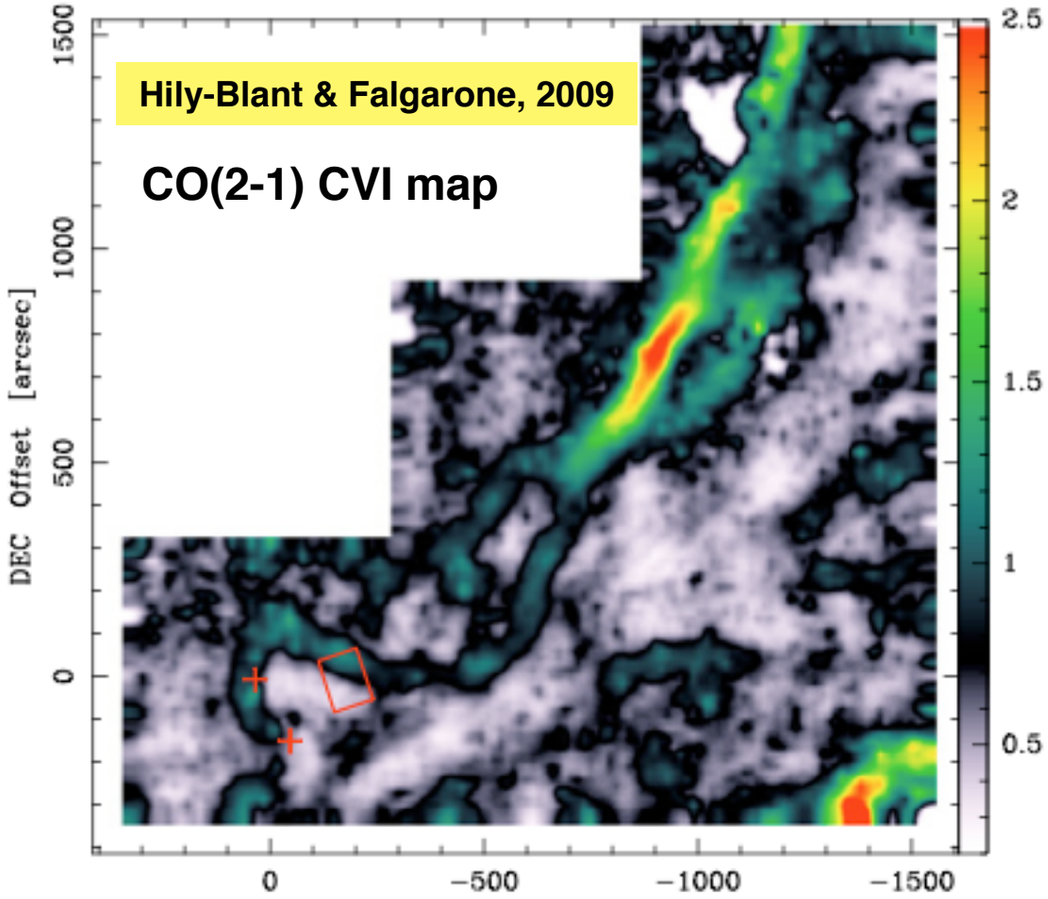
Taurus

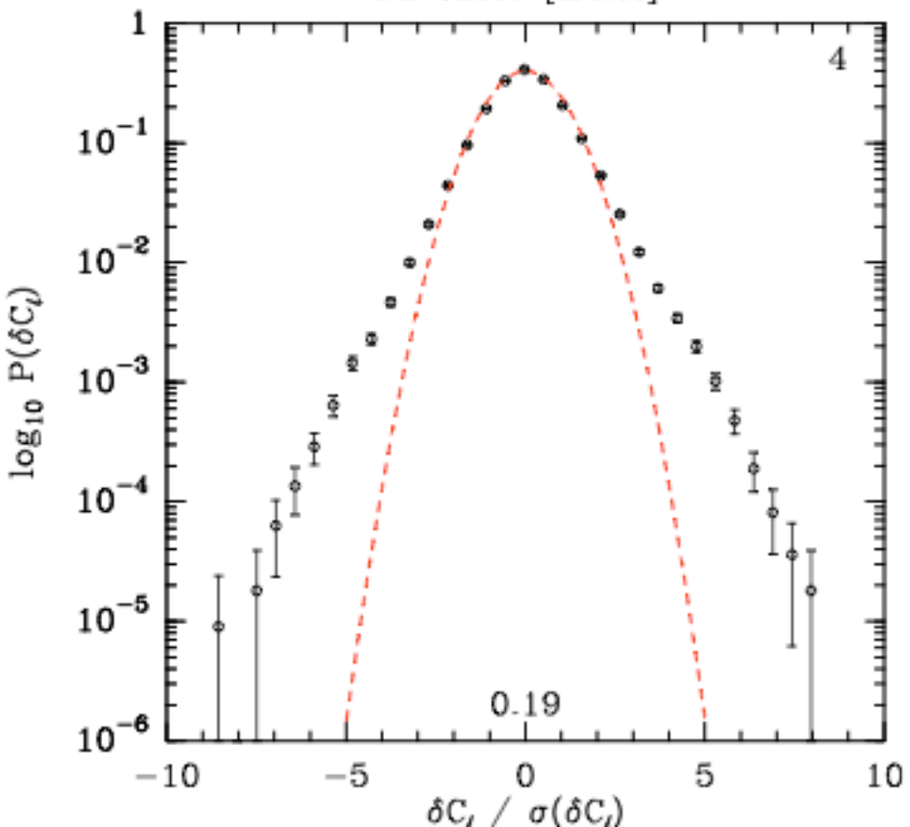


Loci of extreme CVI

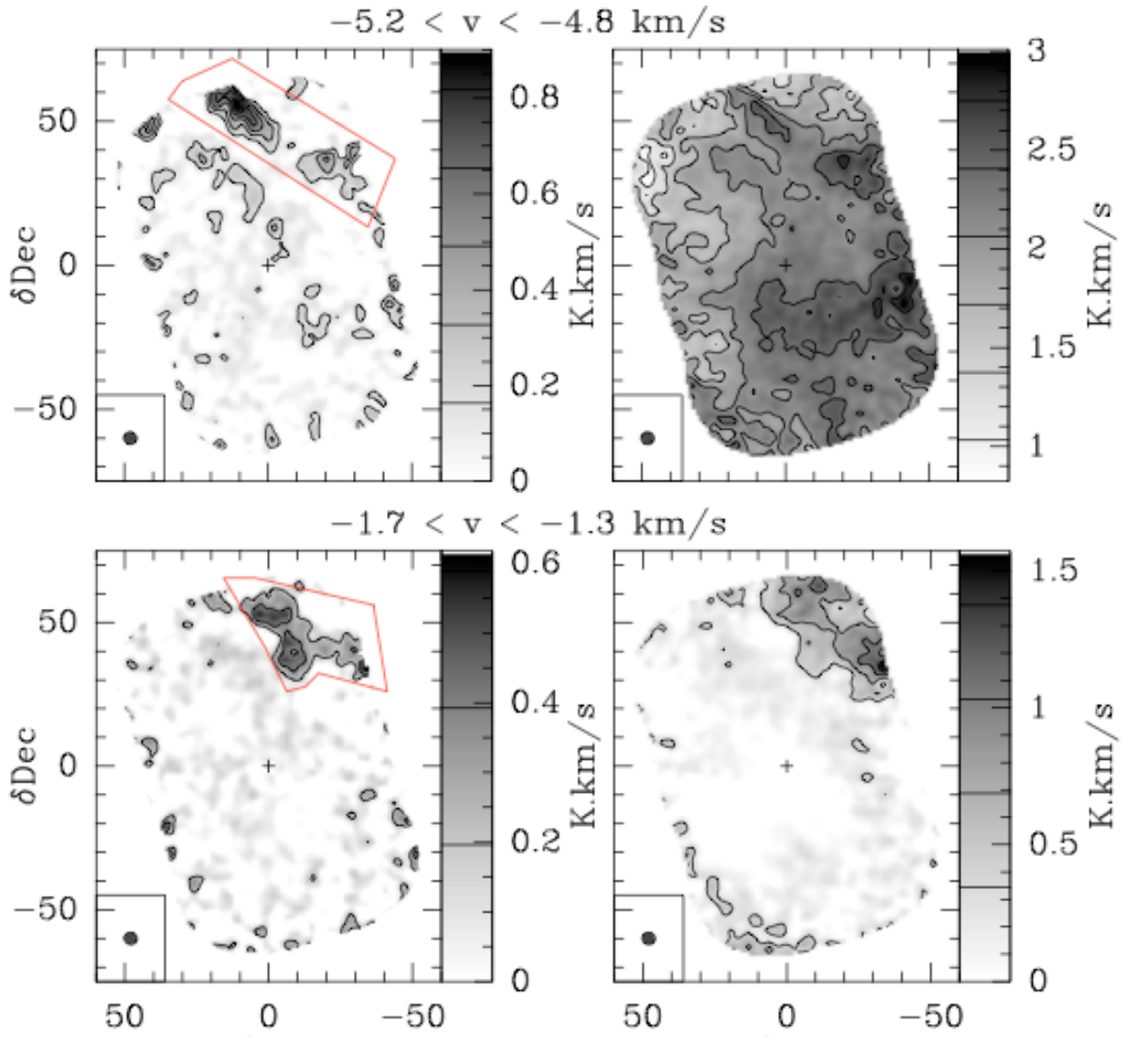
Hily-Blant & Falgarone, 2009

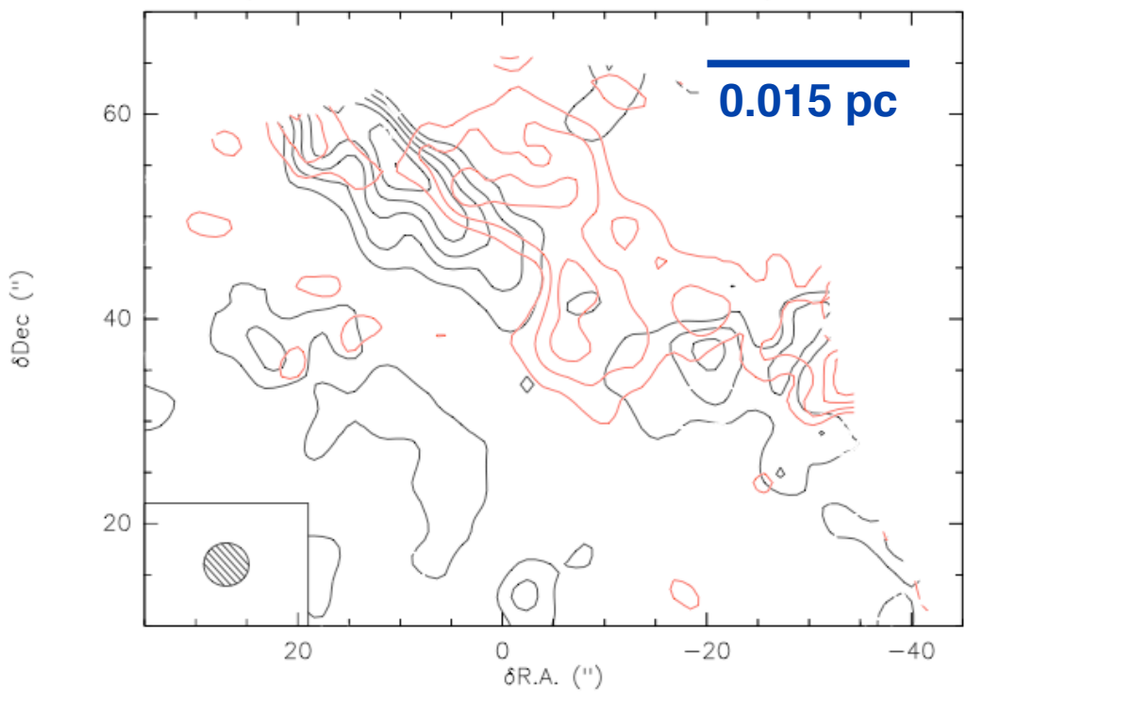
CO(2-1) CVI map





Falgarone, Pety & Hily-Blant, 2009





Aspects of ISM modeling

A variety of processes requiring a variety of modeling tools…

- **Self-gravity**
- **(Magneto)hydrodynamics**
- **Chemical evolution**
- **Radiative transfer**
- **Instrumental effects**

ZEUS began as a hydrodynamics code written by Mike Norman for his thesis work with Jim Wilson in the late 1970s. David Clarke made substantial modifications and improvements in the early 1980s, and coined the name "ZEUS". In the late 1980s, Jim Stone rewrote the code to introduce a covariant differencing formalism, to add new algorithms for MHD and radiation hydrodynamics, and to port it to the UNIX operating system. This rewritten code was called ZEUS-2D. Subsequently, David Clarke re-wrote the code again to extend it to 3D. Thus, there are two quite different versions of the code (ZEUS-2D and ZEUS-3D) which incorporate fundamentally the same algorithms, but differ in many details. More recently, Mike Norman's group at UCSD have developed an MPI version called ZEUS-MP.
The original versions of ZEUS were written as part of the Ph.D. thesis research of Mike Norman's students to study the propagation of extragalactic jets (Clarke), and the dynamics of protostellar disks and outflows (Stone). It was Mike Norman's vision to distribute the code freely to the community; since then ZEUS has been used for hundreds of applications in astrophysics.

GADGET is a freely available code for cosmological N-body/SPH simulations on massively parallel computers with distributed memory. **GADGET** uses an explicit communication model that is implemented with the standardized MPI communication interface. The code can be run on essentially all supercomputer systems presently in use, including clusters of workstations or individual PCs.
GADGET computes gravitational forces with a hierarchical tree algorithm (optionally in combination with a particle-mesh scheme for long-range gravitational forces) and represents fluids by means of smoothed particle hydrodynamics (SPH). The code can be used for studies of isolated systems, or for simulations that include the cosmological expansion of space, both with or without periodic boundary conditions. In all these types of simulations, **GADGET** follows the evolution of a self-gravitating collisionless N-body system, and allows gas dynamics to be optionally included. Both the force computation and the time stepping of **GADGET** are fully adaptive, with a dynamic range which is, in principle, unlimited. **GADGET** can therefore be used to address a wide array of astrophysically interesting problems, ranging from colliding and merging galaxies, to the formation of large-scale structure in the Universe. With the inclusion of additional physical processes such as radiative cooling and heating, **GADGET** can also be used to study the dynamics of the gaseous intergalactic medium, or to address star formation and its regulation by feedback processes.

Enzo is a community-developed adaptive mesh refinement simulation code, designed for rich, multi-physics hydrodynamic astrophysical calculations.
Enzo is freely available, developed in the open, with a strong support structure for assistance. Simulations conducted with Enzo have been featured in numerous refereed journal articles, and it is capable of running on computers from laptop to Top500.

HERACLES is a 3D hydrodynamical code used to simulate astrophysical fluid flows. It uses a finite volume method on fixed grids to solve the equations hydrodynamics, MHD, radiative transfer and gravity. This software is developed at the Service d'Astrophysique, CEA/Saclay as part of the COAST project and registered under the CeCILL license.

The code is developed by:
- Code architecture: Edouard Audit
- Parallelization: Edouard Audit
- Hydrodynamics: Edouard Audit
- Radiative transfer: Matthias González, Edouard Audit & Neil Vaytet
- MHD: Sebastien Fromang, Patrick Hennebelle & Romain Teyssier
- Gravity: Pascal Tremblin
- HDF5 output: Bruno Thooris
- Website: Neil Vaytet

The simulation code **GIZMO** is a flexible, multi-method magneto-hydrodynamics+gravity code. The code lets you solve the hydrodynamic equations using a variety of different methods -- whatever is best for the problem at hand. In particular, it introduces a couple of new, Lagrangian Godunov-type methods, that allow you to solve the fluid equations with a moving particle distribution that is automatically adaptive in resolution and avoids the advection errors, angular momentum conservation errors, and excessive diffusion problems that seriously limit the applicability of “adaptive mesh” (AMR) codes, while simultaneously avoiding the low-order errors inherent to simpler methods like smoothed-particle hydrodynamics (SPH). But, if you want to use SPH -- either in “traditional” form or “modern” (more accurate) forms, or use a mesh, you can do that too with **GIZMO**! Meanwhile, self-gravity is solved fast, with a BH-Tree (optionally a hybrid PM-Tree for periodic boundaries), and on-the-fly adaptive gravitational softenings.
The code is descended from P-GADGET, itself descended from GADGET-2, and many of the naming conventions remain (for the sake of compatibility with the large library of GADGET work and analysis software). Currently available modules include things like: hydrodynamics, MHD (ideal and non-ideal), radiation transport, cosmological integrations, galaxy/star/black hole formation with feedback from stars and black holes (both explicit, detailed models and sub-grid models), self-interacting dark matter, adaptive gravitational softening lengths for all particle types, anisotropic conduction & viscosity, sub-grid turbulent diffusion, the ability to insert arbitrary external gravitational fields, integration in non-standard cosmologies, sink particles, "dust fluids" (particulate-gas interactions), cosmic rays, nuclear+degenerate equations of state (in progress, partially implemented).
No, the code title is not an acronym, I just liked it. It refers both to the code's multi-purpose applications and to its historical relation ship to GADGET.

We also provide a code, named Nahoon, to study the time- dependent gas-phase chemistry of 0D and 1D interstellar sources.

Cholla : A New Massively-Parallel Hydrodynamics Code For Astrophysical Simulation

Fervent: Chemistry-coupled, ionising and non-ionising radiative feedback in magnetohydrodynamical simulations

C. Baczynski, S. C. O. Glover, R. S. Klessen

(Submitted on 31 Mar 2015)

We introduce a radiative transfer code module for the magnetohydrodynamical adaptive mesh refinement code FLASH 4. It is coupled to an efficient chemical network which explicitly tracks the three hydrogen species H, H_2, H+ as well as C+ and CO. The module is geared towards modeling all relevant thermal feedback processes of massive stars, and is able to follow the non-equilibrium time-dependent thermal and chemical state of the present-day interstellar medium as well as that of dense molecular clouds. We describe in detail the implementation of all relevant thermal stellar feedback mechanisms, i.e. photoelectric, photoionization and H_2 dissociation heating as well as pumping of molecular hydrogen by UV photons. All included radiative feedback processes are extensively tested. We also compare our module to dedicated photon-dominated region (PDR) codes and find good agreement in our modeled hydrogen species once our radiative transfer solution reaches equilibrium. In addition, we show that the implemented radiative feedback physics is insensitive to the spatial resolution of the code and show under which conditions it is possible to obtain well-converged evolution in time. Finally, we briefly explore the robustness of our scheme for treating combined ionizing and non-ionizing radiation.

Athena is a grid-based code for astrophysical magnetohydrodynamics (MHD). It was developed primarily for studies of the interstellar medium, star formation, and accretion flows. Athena has been made freely available to the community in the hope that others may find it useful.

The current version (v4.2) implements algorithms for the following physics:

- compressible hydrodynamics and MHD in 1D, 2D, and 3D,
- special relativistic hydrodynamics and MHD,
- ideal gas equation of state with arbitrary γ (including $\gamma = 1$, an isothermal EOS),
- an arbitrary number of passive scalars advected with the flow,
- self-gravity, and/or a static gravitational potential,
- Ohmic resistivity, ambipolar diffusion, and the Hall effect,
- both Navier-Stokes and anisotropic (Braginskii) viscosity,
- both isotropic and anisotropic thermal conduction,
- optically-thin radiative cooling.

PLUTO is a freely-distributed software for the numerical solution of mixed hyperbolic/parabolic systems of partial differential equations (conservation laws) targeting high Mach number flows in astrophysical fluid dynamics. The code is designed with a modular and flexible structure whereby different numerical algorithms can be separately combined to solve systems of conservation laws using the finite volume or finite difference approach based on Godunov-type schemes.

AZEuS: Adaptive Zone Eulerian Scheme¶

AZEuS is a block-based adaptive mesh refinement (AMR) magnetohydrodynamics (MHD) astrophysical fluid code which employs the staggered-mesh ZEUS-3D as its underlying method (Clarke, 1996, 2010; ZEUS-3D website).

Abstract¶

All astrophysical AMR fluid codes in use today are based on a zone-centred method, with all hydrodynamical variables (density, energy, and momentum components) located at the centres of their respective zones. AMR MHD solvers are designed with either zone-centred or face-centred magnetic field components, depending, in part, on the mechanism used to preserve the solenoidal condition. One such scheme is Constrained Transport (CT; Evans & Hawley, 1988), which locates magnetic field components at the centres of the zone-faces to which they are normal. The staggered mesh introduced in such a scheme must be accounted for in the AMR in such a way that the solenoidal condition remains zero everywhere – including within the boundaries – to machine round-off error (e.g., Balsara, 2001; Li & Li, 2004).
One of the few astrophysical fluid codes in wide use that employ a fully-staggered grid, where the momentum components are face-centred like the magnetic fields, are the ZEUS family of codes. In order to couple ZEUS with AMR and produce AZEuS, the block-based scheme of Berger & Colella (1989) was modified for the fully-staggered mesh, including the proper treatment of face-centred magnetic fields and face-centred momentum.
AZEuS is currently capable of solving problems in 1-D, 2-D, and 3-D in Cartesian, spherical polar, and cylindrical coordinates in both single grid and AMR modes. Physical regimes currently available are: hydrodynamics (HD), ideal MHD, and radiation hydrodynamics (RHD; with flux-limited diffusion [FLD] and a simple ray-tracer). As with all ZEUS-type codes, additional physics modules are easily added. The EDITOR pre-compiler software is also (still) used, which, among other things, provides for auto-parallelisation on shared-memory architectures (i.e., OpenMP).

This is a summary of the 2013 release of the plasma simulation code Cloudy. Cloudy models the ionization, chemical, and thermal state of material that may be exposed to an external radiation field or other source of heating, and predicts observables such as emission and absorption spectra. It works in terms of elementary processes, so is not limited to any particular temperature or density regime. This paper summarizes advances made since the last major review in 1998. Much of the recent development has emphasized dusty molecular environments, improvements to the ionization / chemistry solvers, and how atomic and molecular data are used. We present two types of simulations to demonstrate the capability of the code. We consider a molecular cloud irradiated by an X-ray source such as an Active Nucleus and show how treating EUV recombination lines and the full SED affects the observed spectrum. A second example illustrates the very wide range of particle and radiation density that can be considered.

SHAPE[1] is an interactive 3-D software tool for modelling com- plex gaseous nebulae (mainly planetary nebulae, but also su- pernova remnants, light echoes, emission nebulae from mas- sive stars, high-energy phenomena, etc). The distribution of density, velocity, and other physical properties is generated in- teractively using 3-D mesh structures and other graphical and mathematical tools. From these data the program generates synthetic images, position-velocity diagrams, 1-D spectral pro- files, and channel maps for direct comparison with observa- tions. Its versatility has made it a standard tool for the 3- D reconstruction of planetary nebula (e.g. Steffen et al. 2011, Jones et al. 2010) and the analysis of hydrodynamical simu- lations (e.g. Steffen et al. 2009; Vela ´zquez et al. 2011). SHAPE implements radiative transfer solving for atomic species us- ing coefficients from the CHIANTI (Landi et al. 2012), Kurucz (Smith et al. 1996), and NIST (Reader et al. 2012) databases. However, molecular physics in thermalised and non-thermalised cases was not implemented in SHAPE until now. We designed shapemol to fill this gap.

While an earlier version of shapemol worked as a comple- ment to SHAPE v4.5, it has been fully integrated into SHAPE v5. In its present state, shapemol enables radiative transfer in ^{12}CO and ^{13}CO lines. This is done by interpolating the absorption and emission coefficients from a set of pre-generated tables com- puted under the assumption of the LVG approximation.

A two dimensional hydrochemical hybrid code, KM2, is constructed to deal with astrophysical problems that would require coupled hydrodynamical and chemical evolution. The code assumes axisymmetry in cylindrical coordinate system, and consists of two modules: a hydrodynamics module and a chemistry module. The hydrodynamics module solves hydrodynamics using a Godunov-type finite volume scheme and treats included chemical species as passively advected scalars. The chemistry module implicitly solves non-equilibrium chemistry and change of the energy due to thermal processes with transfer of external ultraviolet radiation. Self-shielding effects on photodissociation of CO and H_2 are included. In this introductory paper, the adopted numerical method is presented, along with code verifications using the hydrodynamics module, and a benchmark on the chemistry module with reactions specific to a photon-dominated region (PDR). Finally, as an example of the expected capability, the hydrochemical evolution of a PDR is presented based on the PDR benchmark.

Nautilus : A fast 1D gas-grain chemical model by FH (2008). Based upon the OSU gas-grain chemical model. Updated from gg_osu_2006v1d by RTG/VW. Rate equations fro
Hasegawa & Herbst (1992). Modified rates following Caselli et al. (1998)\n\n Stiff solver for sparse Jacobians: LSODES/ODEPACK (Hindmarsh 1983)\n Turbulent mixing
implemented through first order operator splitting\n

The *STOKES* computer program is a Monte Carlo radiative transfer code for modeling multi-wavelength polarization. It was designed to model astrophysical objects of various geometries and considers polarization induced by electron and dust scattering. If you are interested in polarization and radiative transfer you might want to follow the links on this page to find out more about *STOKES*. The code is freely available for use. We just ask if you publish results based on *STOKES* computations that you refer to the Marin et al. (2012) and Goosmann et al. (2013) paper describing the latest version of the code.

We introduce a new algorithm for the calculation of multidimensional optical depths in approximate radiative transport schemes, equally applicable to neutrinos and photons. Motivated by (but not limited to) neutrino transport in three-dimensional simulations of core-collapse supernovae and neutron star mergers, our method makes no assumptions about the geometry of the matter distribution, apart from expecting optically transparent boundaries.

Methods. Based on local information about opacities, the algorithm figures out an escape route that tends to minimize the optical depth without assuming any pre-defined paths for radiation. Its adaptivity makes it suitable for a variety of astrophysical settings with complicated geometry (e.g., core-collapse supernovae, compact binary mergers, tidal disruptions, star formation, etc.). We implement the MODA algorithm into both a Eulerian hydrodynamics code with a fixed, uniform grid and into an SPH code where we make use a tree structure that is otherwise used for searching neighbours and calculating gravity.

Results. In a series of numerical experiments, we compare the MODA results with analytically known solutions. We also use snap- shots from actual 3D simulations and compare the results of MODA with those obtained with other methods such as the global and local ray-by-ray method. It turns out that MODA achieves excellent accuracy at a moderate computational cost. In an appendix we also discuss implementation details and parallelization strategies.

http://www.kromepackage.org

Modeling : PdR, XDR, LVG…
ISM in galaxies

Hyperion**

Robitaille 2011

Athena ⟶ Hyperion*

Stone et al. 2008 *Skinner & Ostriker 2013*

http://www.astro.uni-koeln.de/sites/default/files/Zermatt2015/talks/Daniel_Seifried_Talk.pdf

For reference, we provide a short overview of some available radiation hydrodynamics codes and compare individual aspects of the numerical schemes with our new interface.

For instance, Owen et al. (2010) coupled the 3D photoion- ization and radiative transfer code MOCASSIN (Ercolano et al. 2003) with the hydrodynamic code ZEUS-2D (Stone & Norman 1992). MOCASSIN and CLOUDY are similarly extensive equi- librium photoionization solvers, but the temperature parameteri- zation used by Owen et al. is only valid for X-ray heating.

Another example for coupling a microphysical equilibrium solver to a hydrodynamic simulation is the ionization module for the FLASH code (Fryxell et al. 2000) presented by Rijkhorst et al. (2006) and further improved by Peters et al. (2010). The 3D radiative transfer method is highly efficient in simulations with adaptive mesh refinement on distributed systems, but is com- putationally more demanding than the pseudo-3D scheme used here. A similarly advanced parallel radiative transfer method was introduced by Wise & Abel (2011) into the ENZO code (Bryan & Norman 1997; O'Shea et al. 2004); it is called MORRAY. The non-equilibrium chemistry solver is restricted to hydrogen and helium, however (The Enzo Collaboration et al. 2013).

Shapiro et al. (2004) and predating publications have ex- tended the hydrodynamics code CORAL (Raga et al. 1995) to include radiative transfer and non-equilibrium photoioniza- tion of hydrogen, helium, and metals. The scheme uses a simi- lar pseudo-multidimensional radiative transfer method, but ne- glects X-rays, which is one of our main interests. X-rays are also mostly neglected in the numerical schemes, which have been specifically designed to simulate escaping hot-Jupiter at- mospheres, and the authors focus exclusively on 1D simulations (e.g., Yelle 2004; Tian et al. 2005; García Muñoz 2007; Penz et al. 2008; Murray-Clay et al. 2009; Koskinen et al. 2013).

In comparison, only TPCI solves our need for a photoion- ization hydrodynamics solver including hydrogen, helium, and metals as well as the absorption of EUV and X-ray emission.

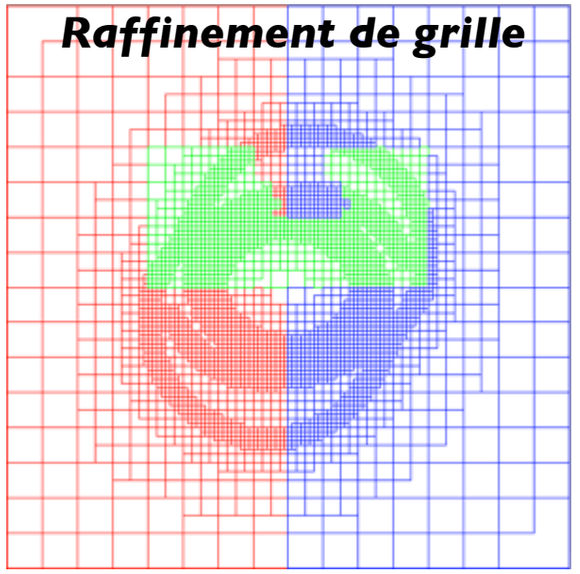
DustEM is a numerical tool that computes the extinction and the emission of interstellar dust grains heated by photons. It is written in fortran 95 and is jointly developed by IAS and IRAP.

The dust emission is calculated in the optically thin limit (no radiative transfer) and the default spectral range is 40 to 108 nm. The code has been designed so that dust properties can easily be changed and mixed and to allow for the inclusion of new grain physics. Data for DustEM is generated by the IDL code **DustProp** which features methods to compute dust optical properties (e.g., Mie, T-matrix, DDA) and heat capacities (internal use only). A description and illustration of DustEM can be found in Compiègne et al (2011).

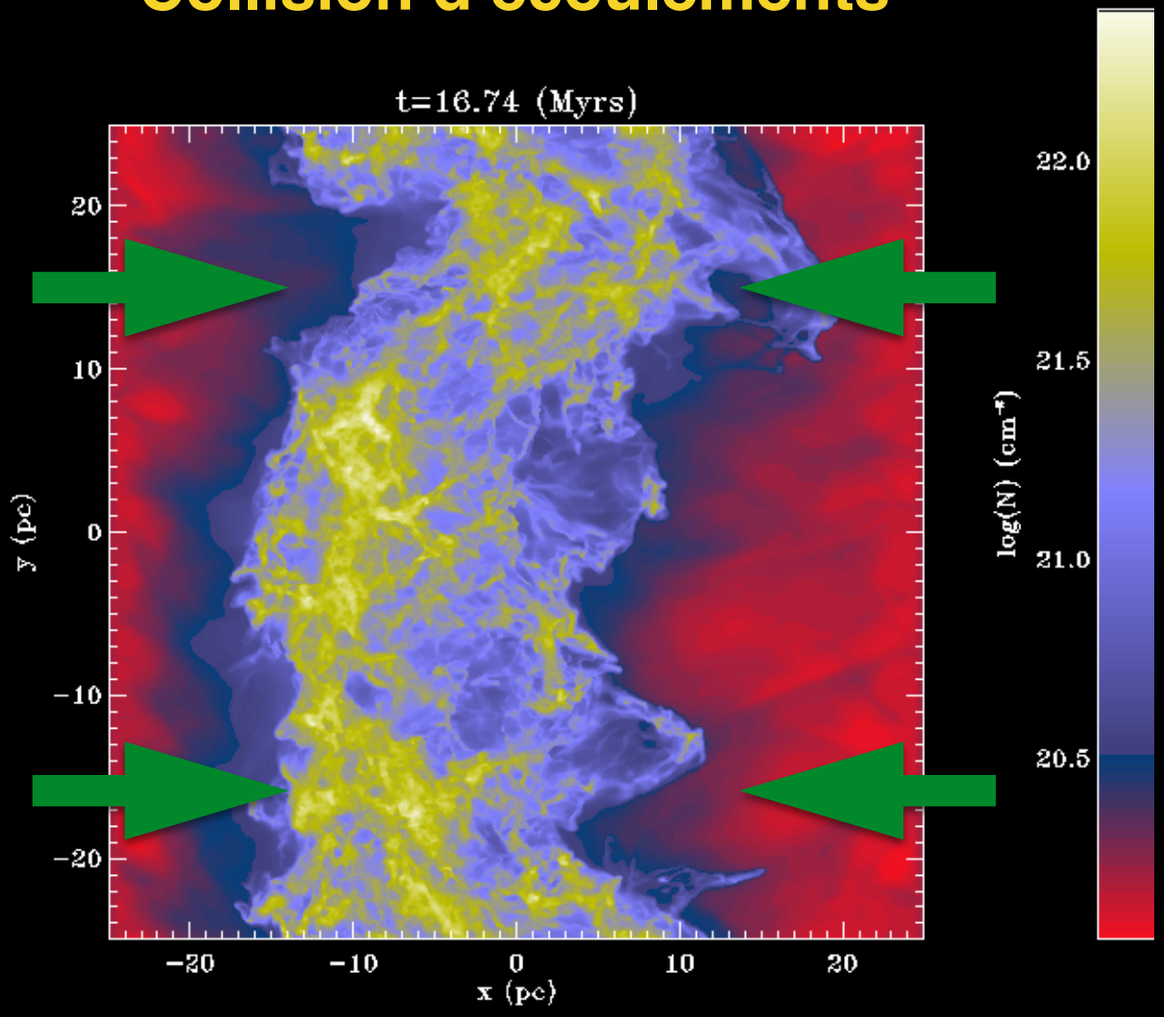
The DustEM Wrapper IDL tool uses DustEM to compute fluxes in a wide range of instrumental bands and to fit dust parameters. DustEM is coupled to the Meudon PDR code where it handles dust physics. DustEM is also coupled to the radiative transfer code CRT of the University of Helsinki as described in Ysard et al. (2012).

Simulations de turbulence MHD

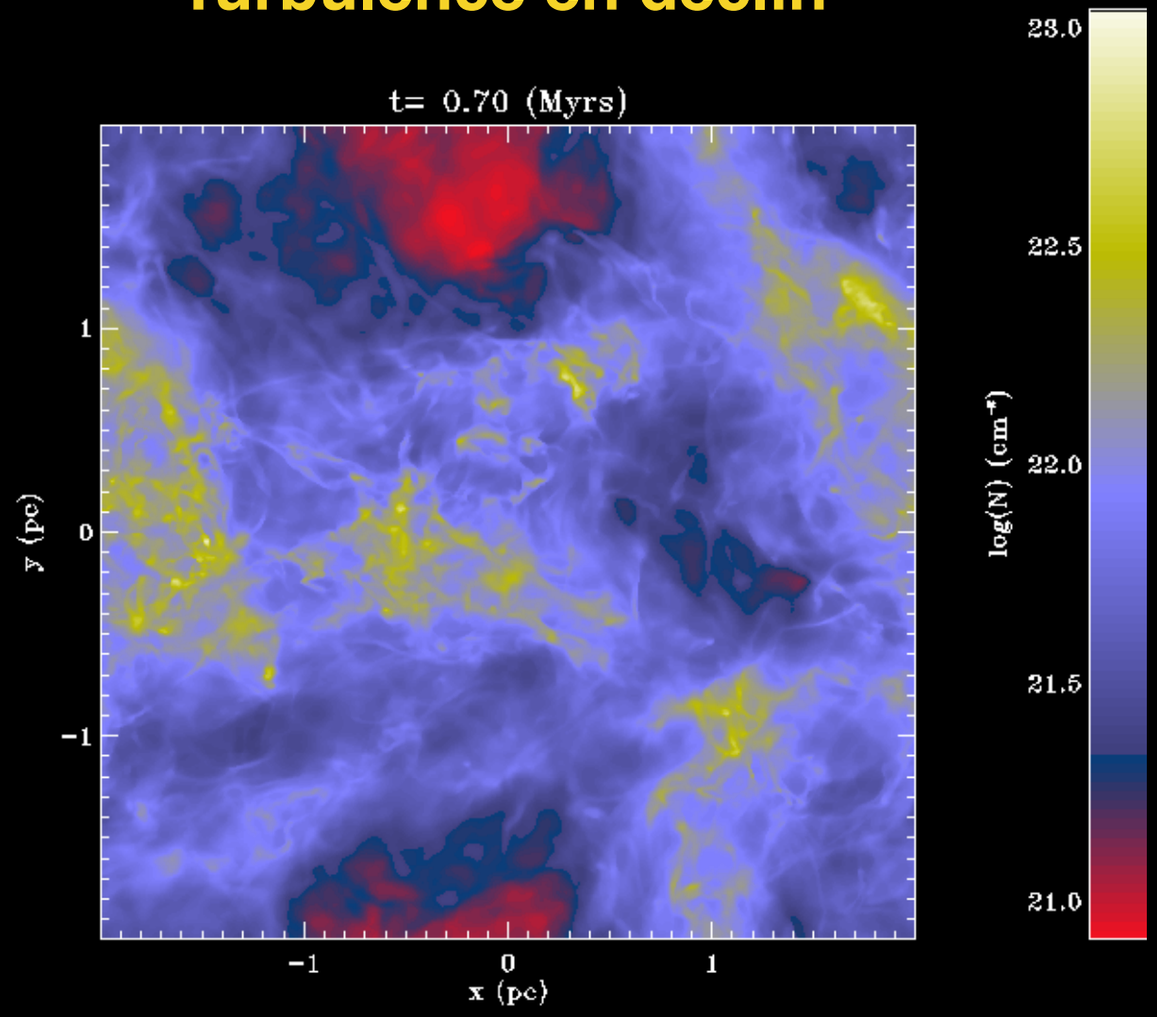
- Code RAMSES code (Teysier 2002, Fromang et al. 2006)
- Raffinement Adaptatif de Maillage (AMR)
- (Magnéto)hydrodynamique
- Autogravitation
- Chauffage et refroidissement du gaz.



Collision d'écoulements



Turbulence en déclin



Cloudy

Ferland et al. 2013

Cloudy initially included the chemistry network described by Black (1978) which was expanded to treat PDRs and XDRs as described by Ferland et al. (1994). Nick Abel carried out a massive upgrade to the heavy-element chemistry network as part of his PhD thesis, described in Abel et al. (2004). Later re- finements are discussed in Abel et al. (2005), Shaw et al. (2005), and Shaw et al. (2006). Appendix A of Abel et al. (2005) gives details of the numerical methods along with differences between UMIST and Cloudy reaction rates. Cloudy had predicted col- umn densities for about 20 heavy element molecules, consisting of C and O atoms. It could not calcu- late physical conditions deep in a PDR or a molec- ular cloud, where most gas phase C, N, and O is in the form of molecules, due to numerical instabilities in the chemistry solver then used. The upgraded chemistry solver has no restrictions, as described in sections below. Cloudy now calculates the chemical abundance of 83 molecules using a network in- cluding ~ 10^3 chemical reactions involving molecules containing H, He, C, N, O, Si, S, and Cl atoms. The network adjusts automatically when elements or species are disabled.

Most reaction rates come from the UMIST 2000 database (Le Teuff et al. 2000) as updated for the Leiden workshop and described by R¨ollig et al. (2007). We also predict the freeze-out of H_2O, CO, and OH on grains, using the data given in Hasegawa & Herbst (1993). Both time-steady and time-dependent chemical evolution calculations are possible.

Cloudy_3D

STOUT

KM2

Cloudy (Ferland et al. 1998; Shaw et al. 2005; Abel et al. 2005), Meudon (Le Bourlot et al. 1993; Le Petit et al. 2006), UCL PDR (Papadopoulos et al. 2002; Bell et al. 2005), Leiden (Black & van Dishoeck 1987; van Dishoeck & Black 1988; Jansen et al. 1995), COSTAR (Kamp & Bertoldi 2000; Kamp & van Zadelhoff 2001), and 3D-PDR (Bisbas et al. 2012), and so on. Comparisons and benchmark studies of these PDR codes were made by Ro¨llig et al. (2007)

Motoyama et al 2015

HELIOS-K: AN ULTRAFAST, OPEN-SOURCE OPACITY CALCULATOR FOR RADIATIVE TRANSFER 12

Draft version June 22, 2015

ABSTRACT

We present an ultrafast opacity calculator that we name HELIOS-K. It takes a line list as an input, computes the shape of each spectral line and provides an option for grouping an enormous number of lines into a manageable number of bins. We implement a combination of Algorithm 916 and Gauss-Hermite quadrature to compute the Voigt profile, write the code in CUDA and optimise the computation for graphics processing unit

Online services

Inverse problems service

ISMServices — PDR Grid Search

Plot axis

x: nH (input parameter) ☐ log scale

y: ISRF scaling factor (observer side) ☐ log scale

Fixed axis

AVmax 0.5

Axis constraints

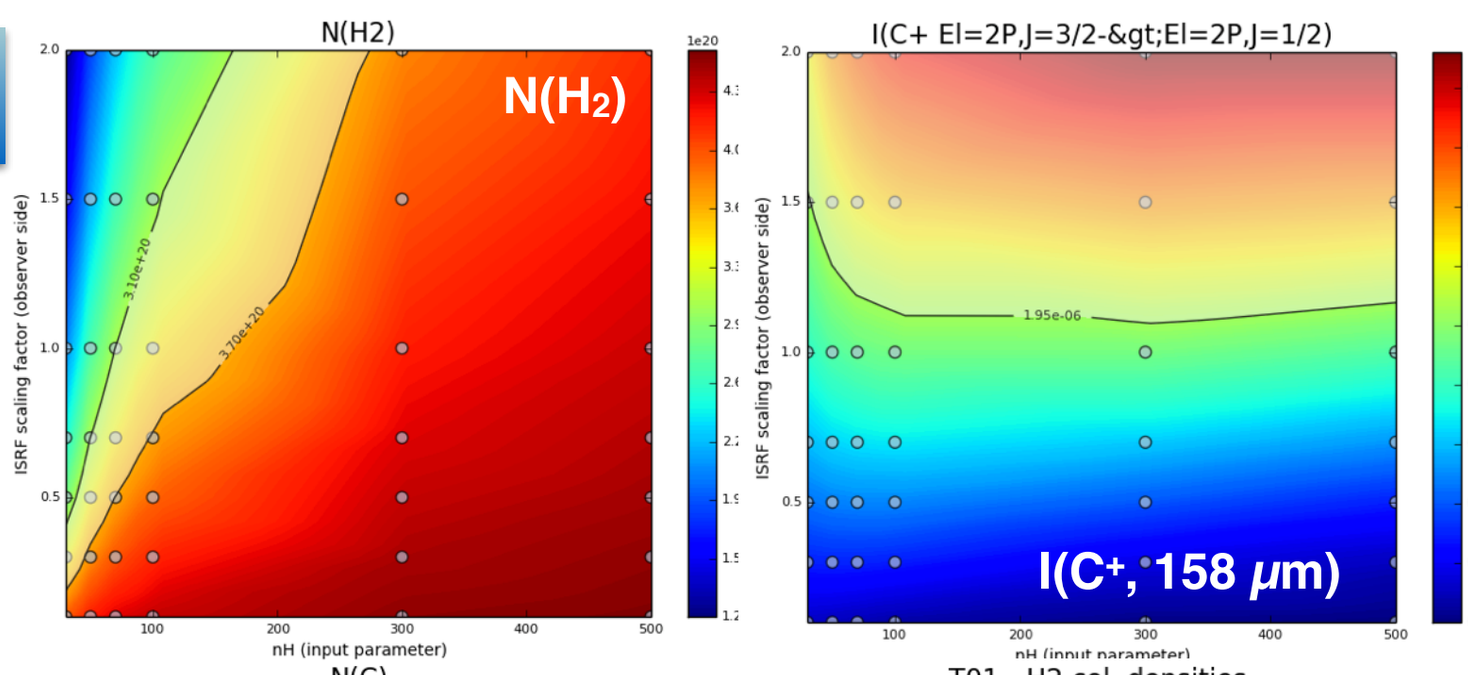
Add ex: X-ray power law slope > -1

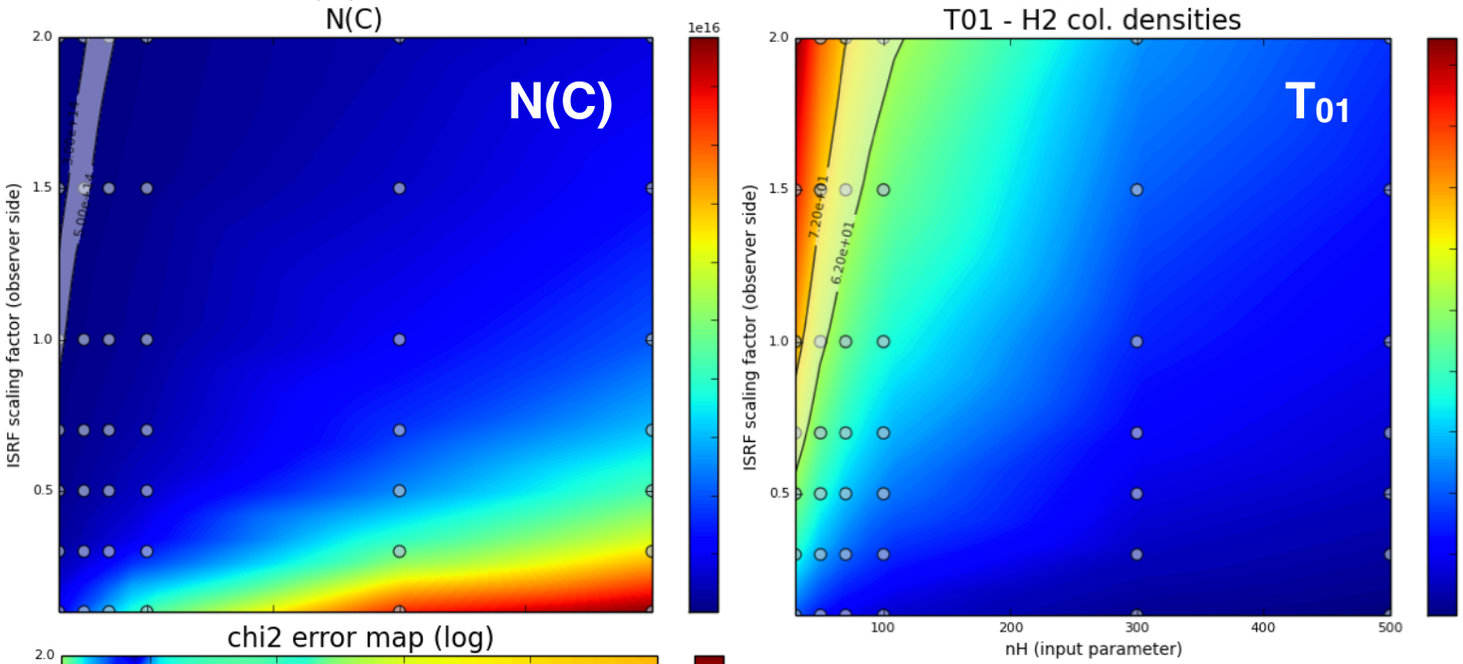
```
N(H2) > 3.1E20
N(H2) < 3.7E20
N(C) > 3.0E14
N(C) < 5.0E14
I(C+ El=2P,J=3/2-&gt;El=2P,J=1/2)  > 1.95E-6
I(C+ El=2P,J=3/2-&gt;El=2P,J=1/2)  < 3.65E-6
```

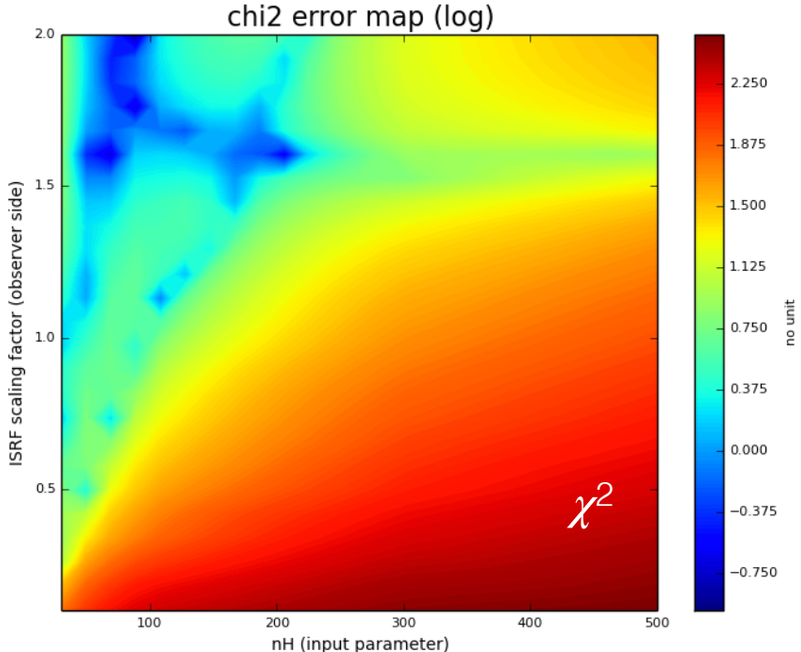
Plot

Query :

3.1E20 <	N(H2)	< 3.7E20
3.0E14 <	N(C)	< 5.0E14
1.9E-6 <	I(C+, 158 µm)	< 3.6E-6
62 <	T01	< 72





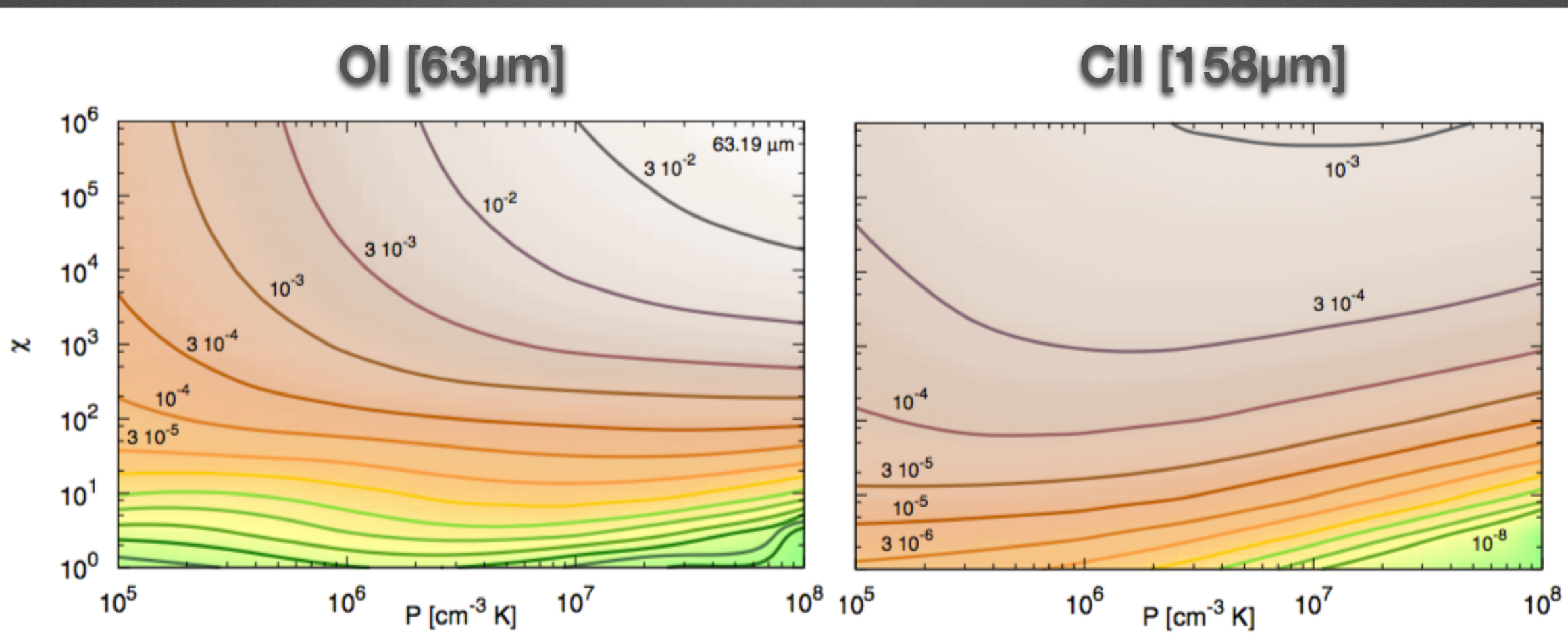


Results :

- n_H ~ 100 cm^{-3}
- G_0 ~ 1.7 Mathis

Example use of the Meudon PDR code

- Isobaric models
- Detailed H_2 formation mechanisms



Le Bourlot et al. 2012

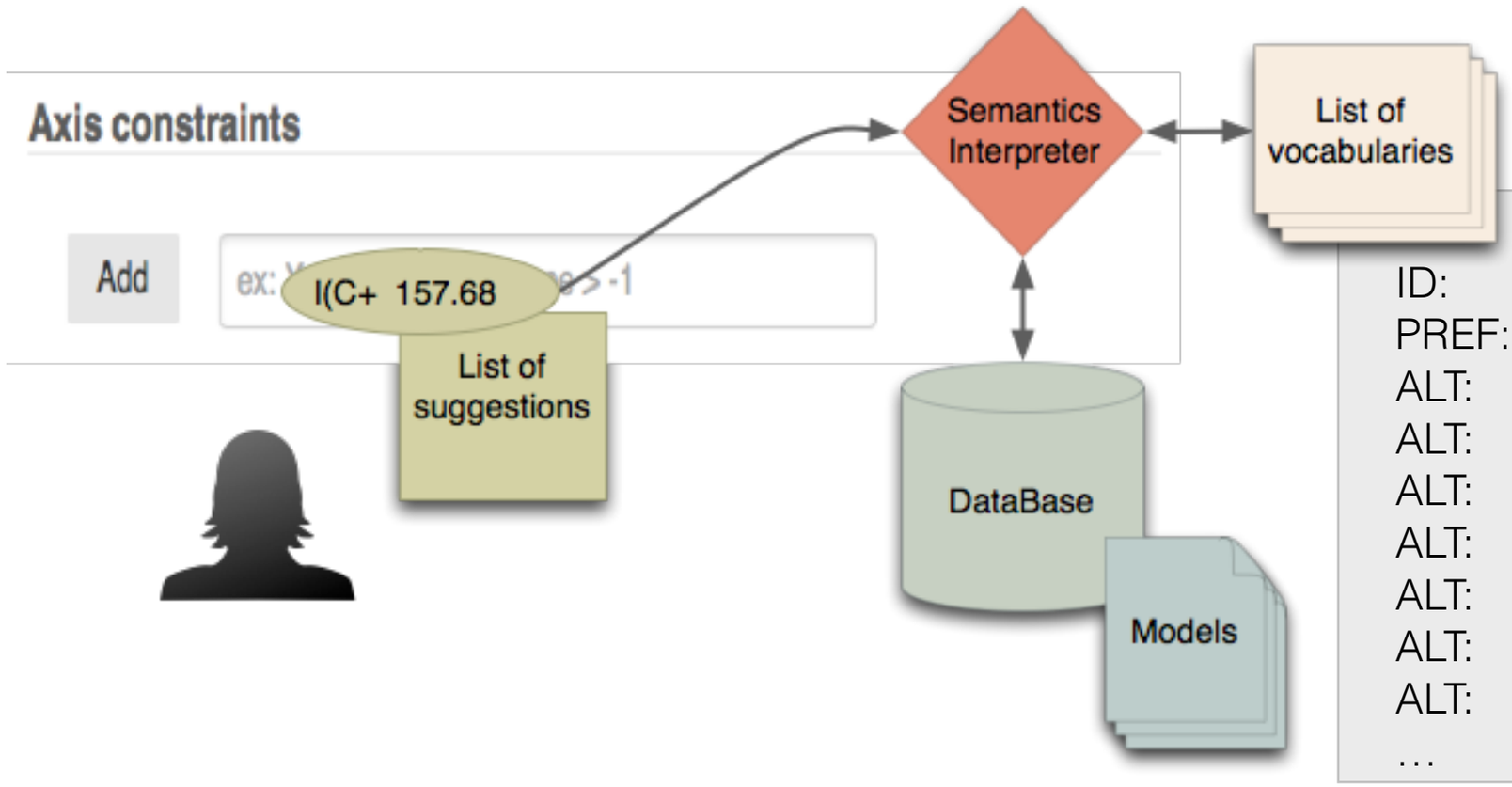
Online services

Intelligent metadata management

- New database technologies to manage so large number of metadata
- Human friendly interface

➔ Web semantics

Simple form :
- Google bar
- Users enter their query in human-like language
- The system interprets the query and understands what it means
- Web semantics / Synonyms



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ALT: I(C+ El=2P,J=3/2->El=2P,J=1/2) face on
ALT: I(C+ 157.68 micron) face on
ALT: Intensity of C+ 157.68 micron face on
ALT: Line intensity of C+ 157.68 micron face on
ALT: I(C+ 1901.2713 GHz) face on
ALT: Intensity of C+ 1901.2713 GHz face on
ALT: Line intensity of C+ 1901.2713 GHz face on
…

Base de données / HDMA / IDA

(D. Languignon, F. Le Petit, E. Bron, B. Godard)

ISMServices

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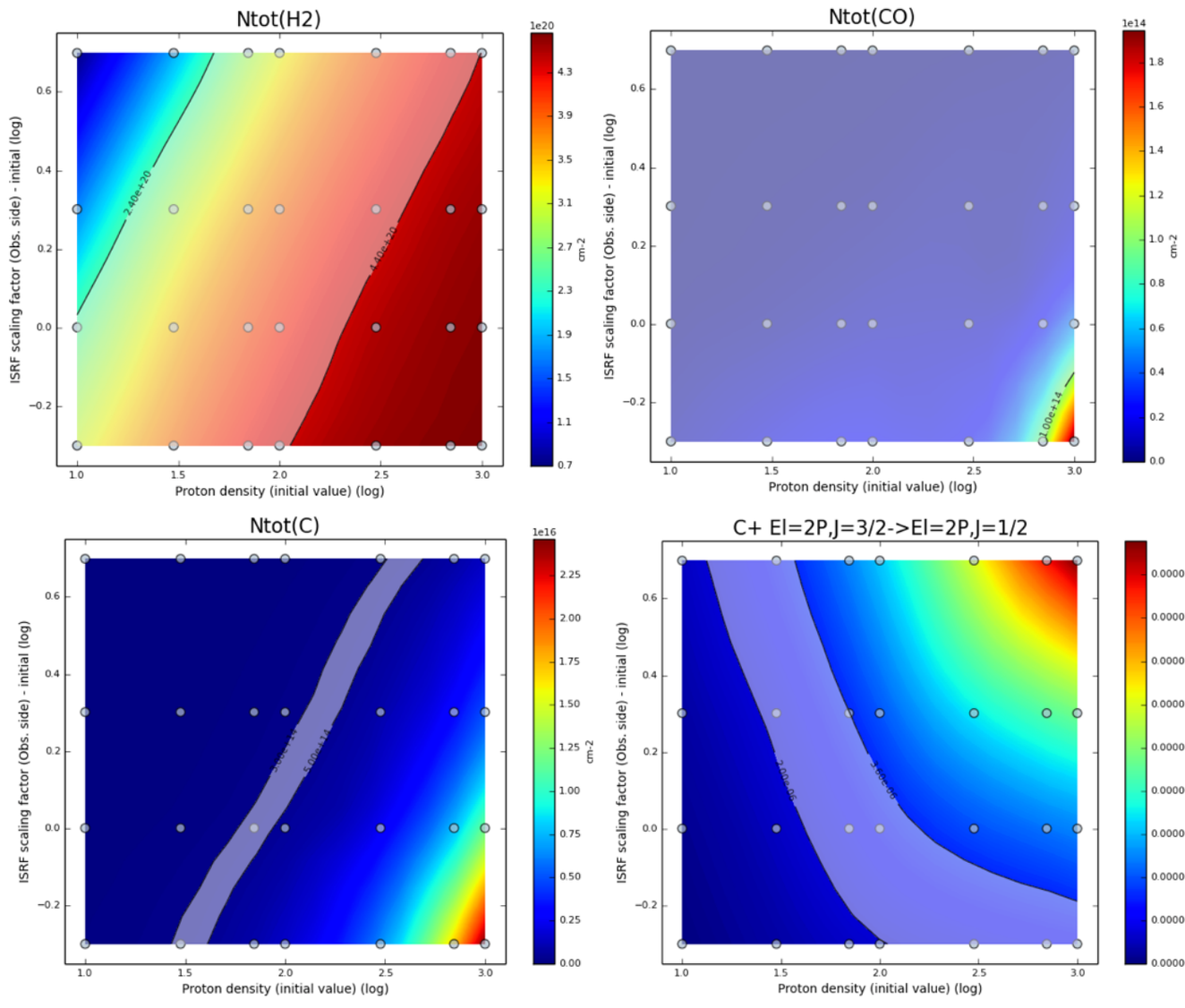
I(C+ El=2P,J=3/2-&gt;El=2P,J=1/2)  < 3.65E-6
```

Plot



Online services

Inverse problems service

Get results in a few minutes instead of weeks / months of work

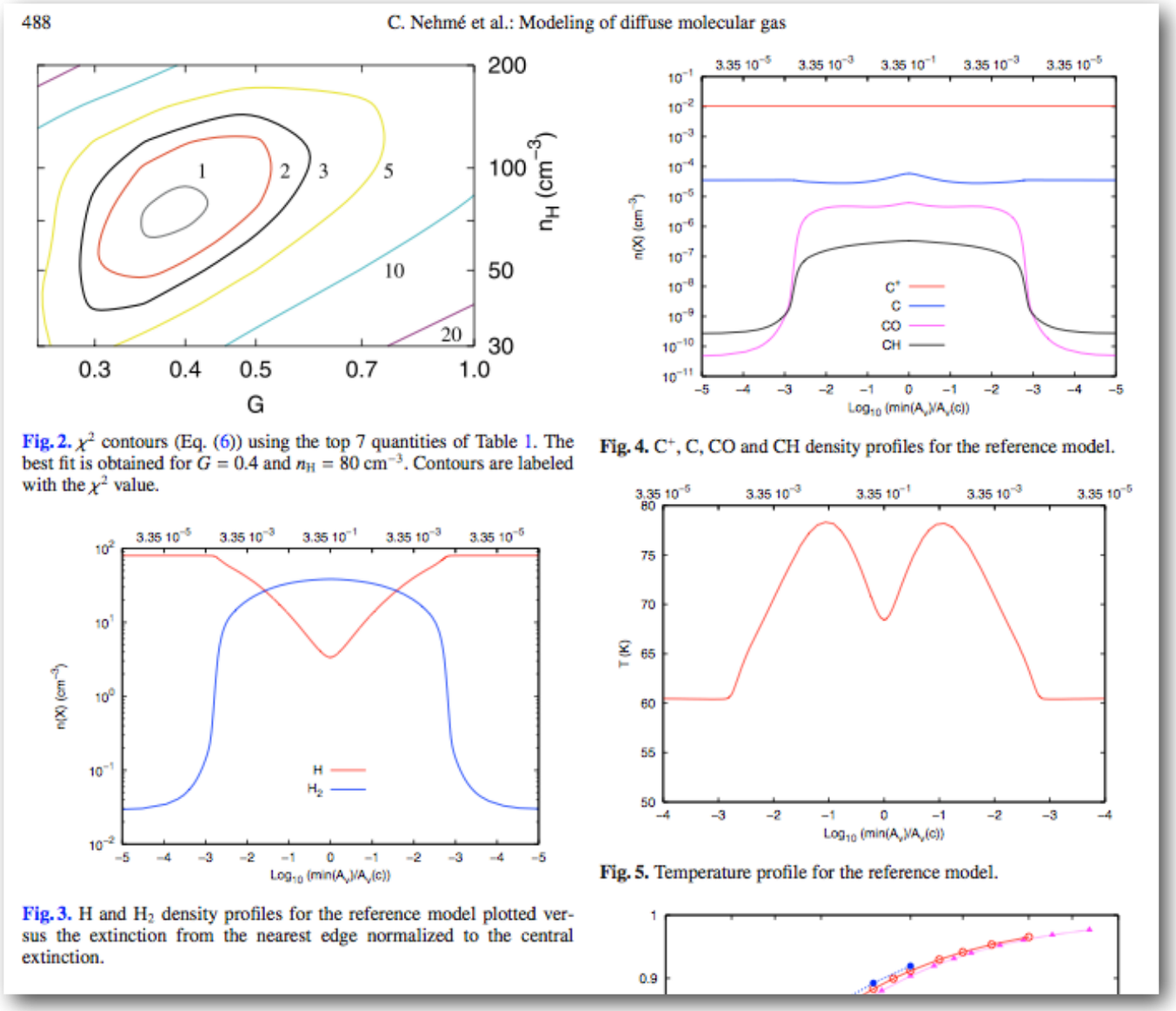


Fig. 2. χ^2 contours (Eq. (6)) using the top 7 quantities of Table 1. The best fit is obtained for $G = 0.4$ and $n_H = 80$ cm^{-3}. Contours are labeled with the χ^2 value.

Fig. 3. H and H_2 density profiles for the reference model plotted versus the extinction from the nearest edge normalized to the central extinction.

Fig. 4. C^+, C, CO and CH density profiles for the reference model.

Fig. 5. Temperature profile for the reference model.

Once one / several models are found :

Functionalities on each model

- Download all models results
- Extraction of some quantities
  - Abundance profiles
  - Temperature profiles
  - Line intensities
  - Column densities
  - Spectra
  - …

Access to the Meudon PDR code

The Meudon PDR is available at:

http://ism.obspm.fr

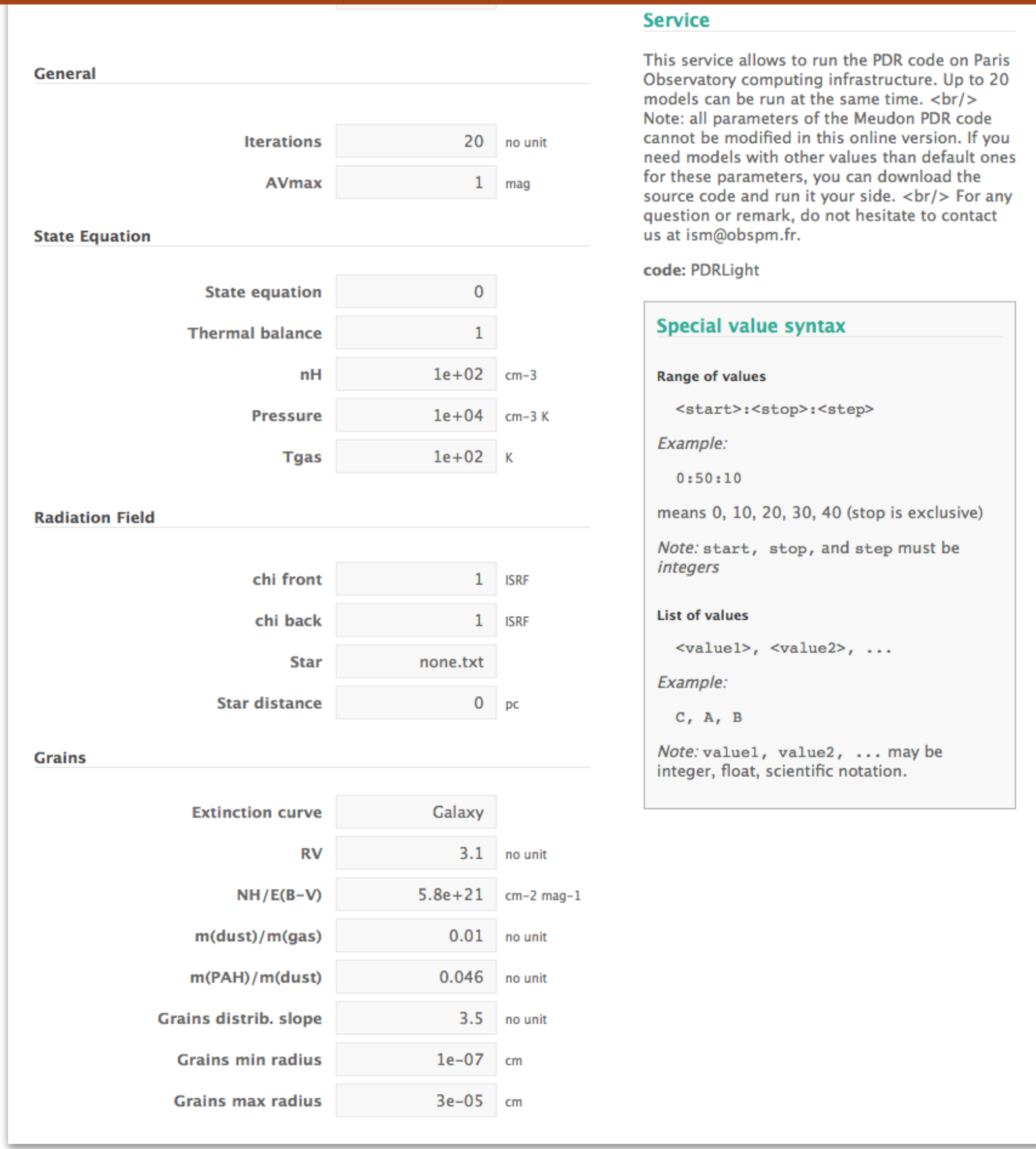
- download source code

Versions

- PDR 1.4.4 (H_2 formation)
- New versions available soon
  - PAH
  - X-rays
  - new physics
  - new atomic & molecular data

Available soon :

- available online with computing ressources at Paris Observatory

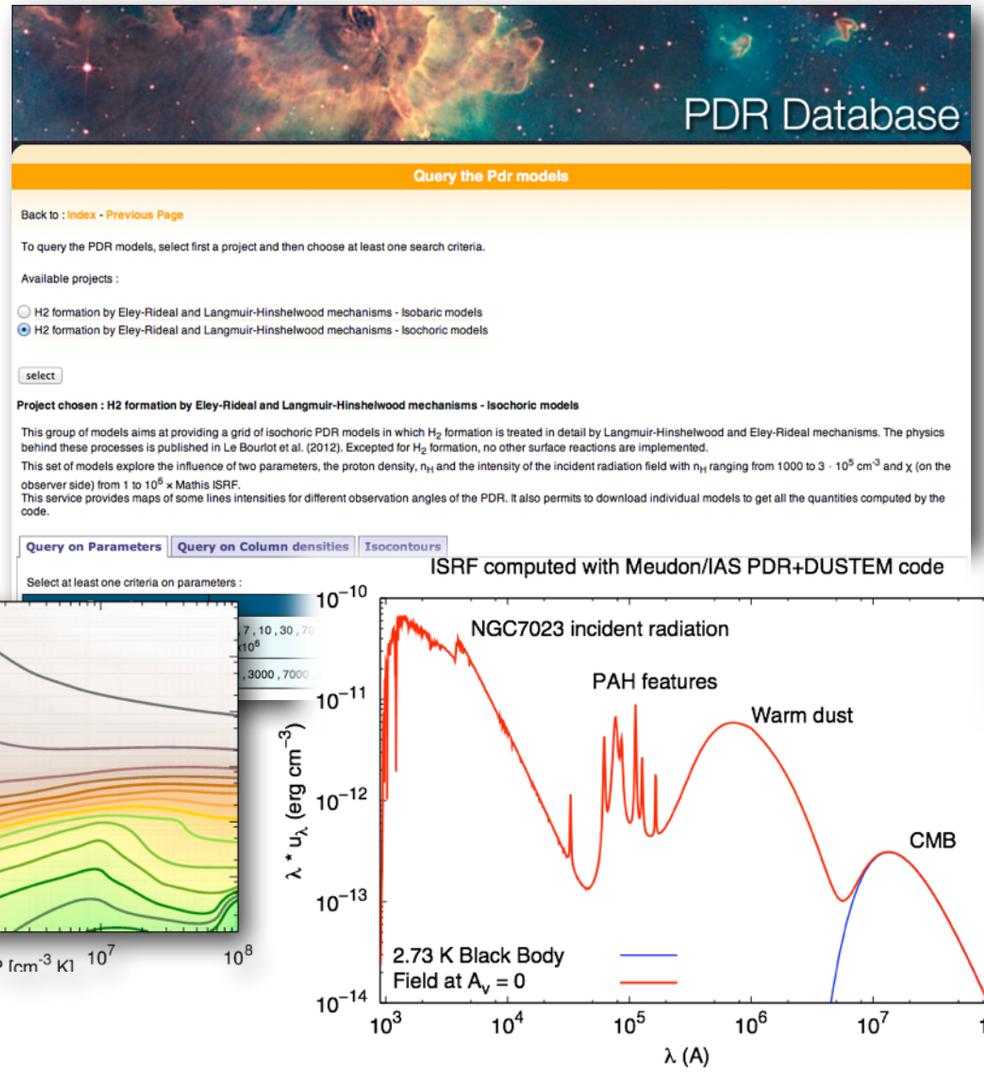


Data bases

PDR Database - version 1

Publish large numbers of pre-computed models
- Diffuse gas
- PDRs
- Dark clouds (with surface chemistry)
- Galactic & Extragalactic ISM

Access to
- column densities & line intensities
- cloud structure (densities, temperature, …)



Starformat (CEA / IRFU - ZAH)
(P. Hennebelle et al.)

- MHD simulations
  - Dense cores & other projects
  - Clumps : Masse distribution, …
- Post-treatment to compute observables (RADMC-3D)