3D Interstellar Chemo-physical Evolution

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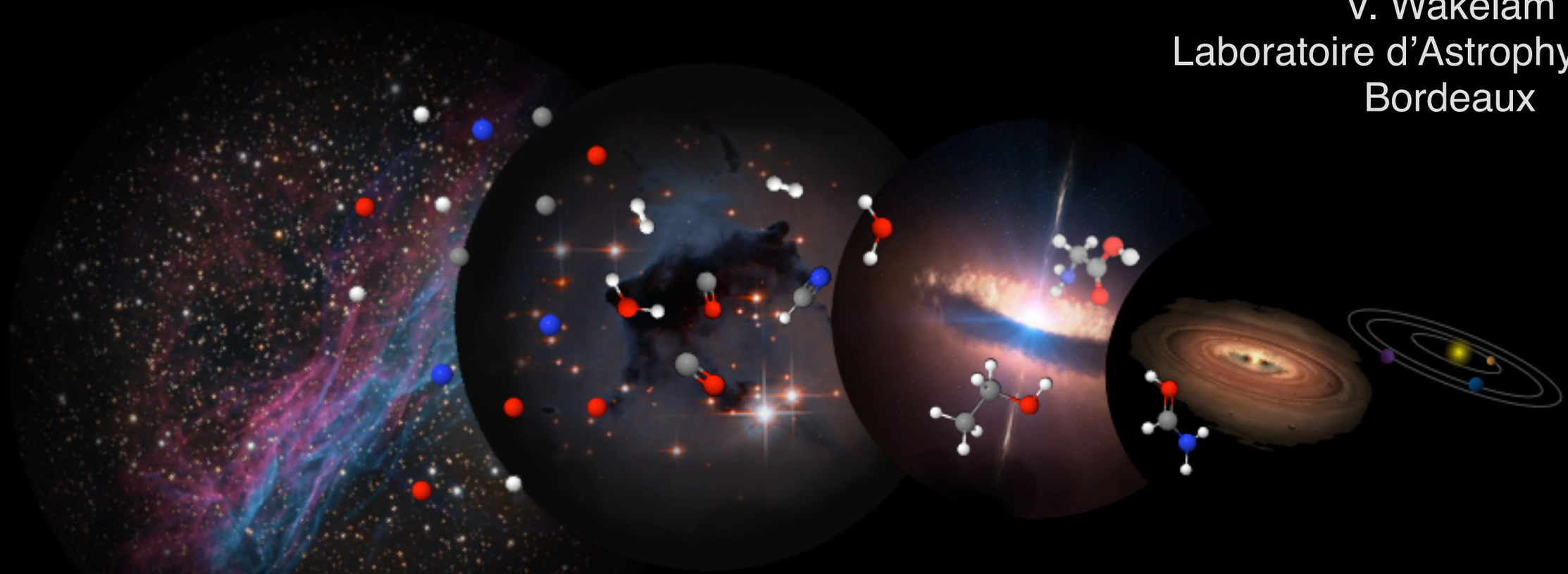
Laboratoire d'Astrophysique de Bordeaux



European Research Council - Starting Grants

- Create a scientific team to work on an identified problem, which could not be solved without an ERC team and needs risky new developments.

- Between 2 to 7 yrs after the PhD defense (between 7 and 12 yr for consolidator grants and senior grants for older)

- In addition to the quality of the project, the success of the grant is based on the PI: his/her ability to find money and his/her independence.

- One call a year

- A lot of money for one person (1.5 millions for up to 5 yr). Example: 5 yrs of postdocs, 2 PhD students, 1 engineer over 3 yr + salary of the PI (at CNRS) given back to the project

- Very positive aspect : we can take time to 1) develop things that are not necessary visible and 2) go deeper.

Example: our gas-grain code Nautilus has been completely modified (work by C. Cossou)

- following the modifications with GIT
- writing notices for users and developers

→ long term survival of the code

→ easier start of new students and postdocs

→ long term perspective: public domain

nautilus

Gas grain chemical model

Search projects

Project Home | Wiki | Issues | **Source** | Administer

Repository: default | Checkout | Browse | **Changes** | Clones | Request code review

Committed Changes Download zip | tar.gz — Oct 14 - Jul 30 Older ›

Rev	Scores	Commit log message	Date	Author
2a36d2a008ef		Few modifications of the documentation. Correction of the format of the line JH2 in the file surfac…	Oct 14, 2014	Valentine Wakelam <wa…
e0f32473cb26		2 *.dat files were missing in the previous push.	Oct 2, 2014	Valentine Wakelam <wa…
ecc0b7f9e6be		Modification of the code to do correctly the self-shielding of CO and H2. The computation of H2 …	Sep 29, 2014	Valentine Wakelam <wa…
e0e4f38278e9		Modification of the test to warn the user when the hydrogen and the helium are too depleted on t…	Sep 25, 2014	Valentine Wakelam <wa…
b392927b3c59		bug fixing: the length of the lines matters !!!! nb_sample_1D changed to spatial_resolution in nau…	Sep 24, 2014	Valentine Wakelam <wa…
08173a2b6165		nb_sample_1D changed to spatial_resolution	Sep 24, 2014	Valentine Wakelam <wa…
88fcf7336a04		1D_evolution changed to 1D_static since the code does not treat 1D evolving physical structure…	Sep 24, 2014	Valentine Wakelam <wa…
7951c4f2b5d1		Merge branch 'master' of https://code.google.com/p/nautilus Just comments added.	Sep 24, 2014	Valentine Wakelam <wa…
6696d83d3d3c		Only comments have been modified.	Sep 24, 2014	Valentine Wakelam <wa…
bf5596dcf956		Fixed progressbar so that it works with logarithmically spaced time intervals	Sep 22, 2014	Pierre Gratier <pierre.gr…
a450182e64a3		correcting missing comment in parameters.in. Seemed not a problem, but just in case.	Sep 19, 2014	Autiwa <autiwa@gmail.…
39cf0b59fadc		update of documentation	Sep 19, 2014	Autiwa <autiwa@gmail.…
12e36c8c8c0d		Adding a structure_type to allow 1D without species diffusion (1D_no_diff)	Sep 19, 2014	Autiwa <autiwa@gmail.…
375b7443bb42		Merge branch 'master' of https://code.google.com/p/nautilus	Sep 18, 2014	Autiwa <autiwa@gmail.…
d062a96e89df		minor changes, including a new paragraph to explain a bit more precisely how the diffusion is …	Sep 18, 2014	Autiwa <autiwa@gmail.…
940acc0c9379		Minor modification in dust_temperature_module.f90	Sep 8, 2014	Maxime Ruaud <maxim…
2c59cfc76f07		Add some references into dust_temperature_module.f90 and correct an expression in the calc…	Sep 8, 2014	Maxime Ruaud <maxim…
901e6611b9af		Modifications in dust_temperature_module.f90. Now we consider a mix of graphite and silicat…	Sep 8, 2014	Maxime Ruaud <maxim…
1caf6376e87e		minor modif in nautilus_profile	Aug 9, 2014	Autiwa <autiwa@gmail.…
4610857c88a0		minor modifs in unitary_tests.py, so that compilation stuff is defined only in Makefile.py	Aug 1, 2014	Autiwa <autiwa@gmail.…
76be7b8cca65		minor modifs	Jul 31, 2014	Christophe Cossou <cc…
90bca281aee2		Merge branch 'master' of https://code.google.com/p/nautilus	Jul 31, 2014	ccossou <cossou@mac…
f74bf8e71bdf		Update of the documentation about the new script	Jul 31, 2014	ccossou <cossou@mac…
cd26c6821041		creation alias for the new binary	Jul 31, 2014	Christophe Cossou <cc…
dfcb6385bb8c		Merge branch 'master' of https://code.google.com/p/nautilus	Jul 30, 2014	ccossou <cossou@mac…

Oct 14 - Jul 30 Older ›

The 3DICE project: scientific context

Strong UV irradiation

Diffuse medium

Depletion of atoms on grains

gas

grain

Dark cloud

Cold gas-phase chemistry
Formation of ices

ice

Warm gas phase chemistry
Modification of ices

Protostar

grain

gas

ice

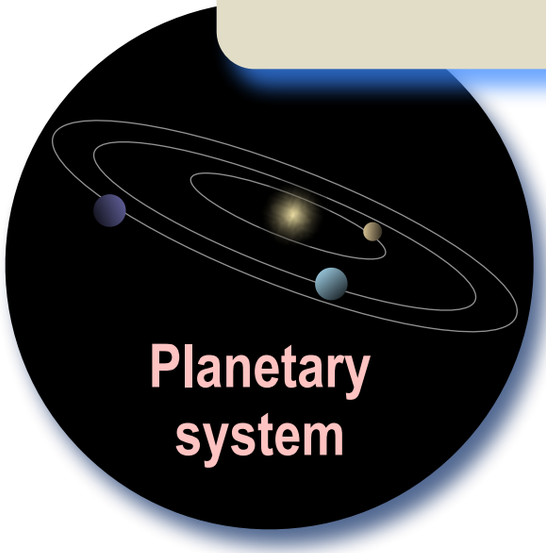
Strong UV field
Coagulation and sedimentation of grains

Protoplanetary disc

Planetary system

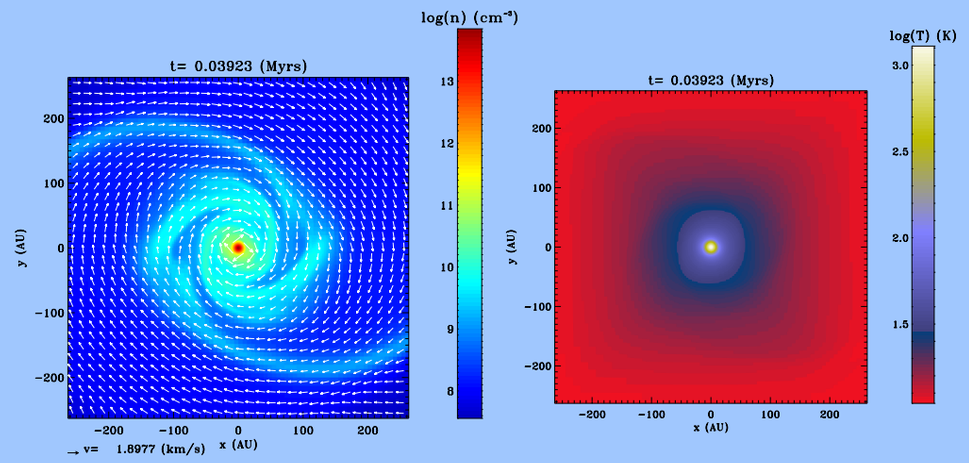
Science case: Interstellar chemical evolution

- Consistent physical scenario
- Better characterisation of the first step



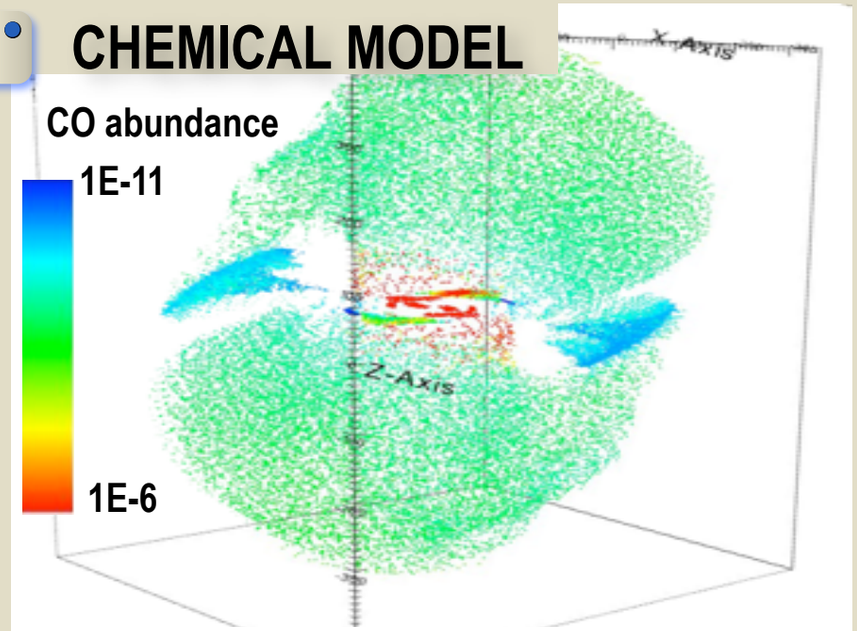
Methodology

3D DYNAMICAL PHYSICAL STRUCTURE



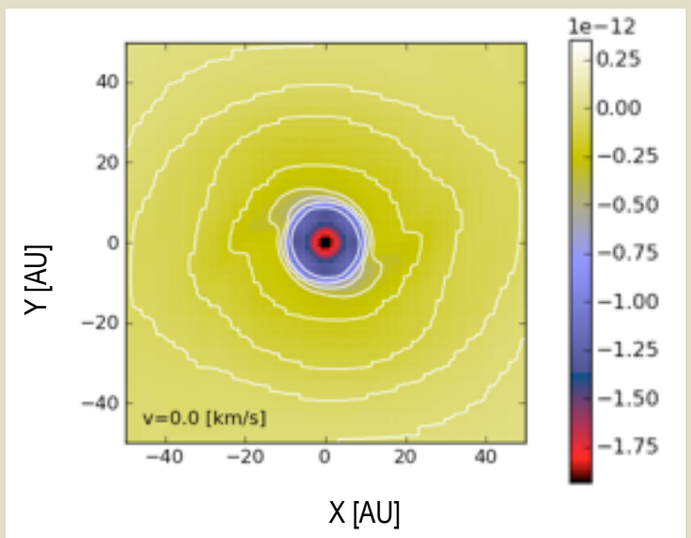
Density Temperature

CHEMICAL MODEL



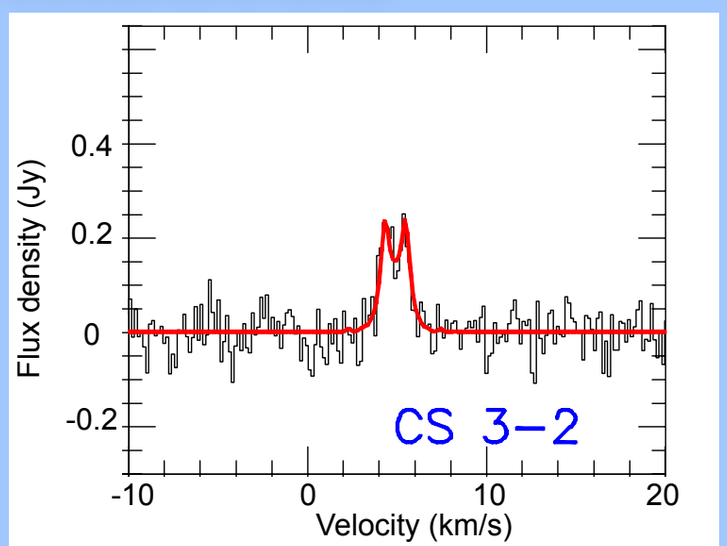
(Hincelin, Wakelam et al. submitted)

3D RADIATIVE TRANSFER



Intensity maps CO (3-2) (Hincelin, Wakelam et al. in prep.)

OBSERVATIONS



Dutrey, Wakelam et al. (2011)

The team

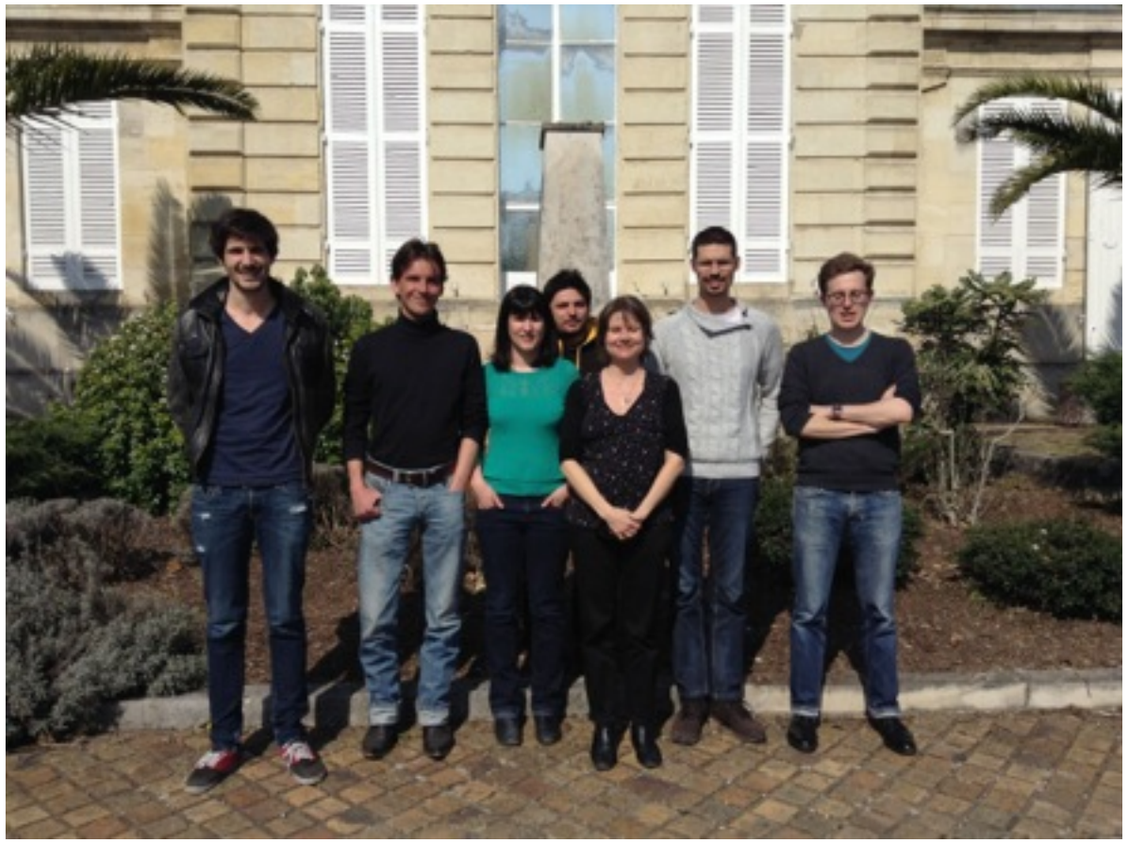
http://www.obs.u-bordeaux1.fr/amor/VWakelam/3DICE

F. Hersant (CNRS)
B. Pavone (3DICE)
P. Gratier (3DICE)
M. Ruaud (3DICE)
L. Reboussin (U. Bord.)

Former member:
C. Cossou (3DICE)

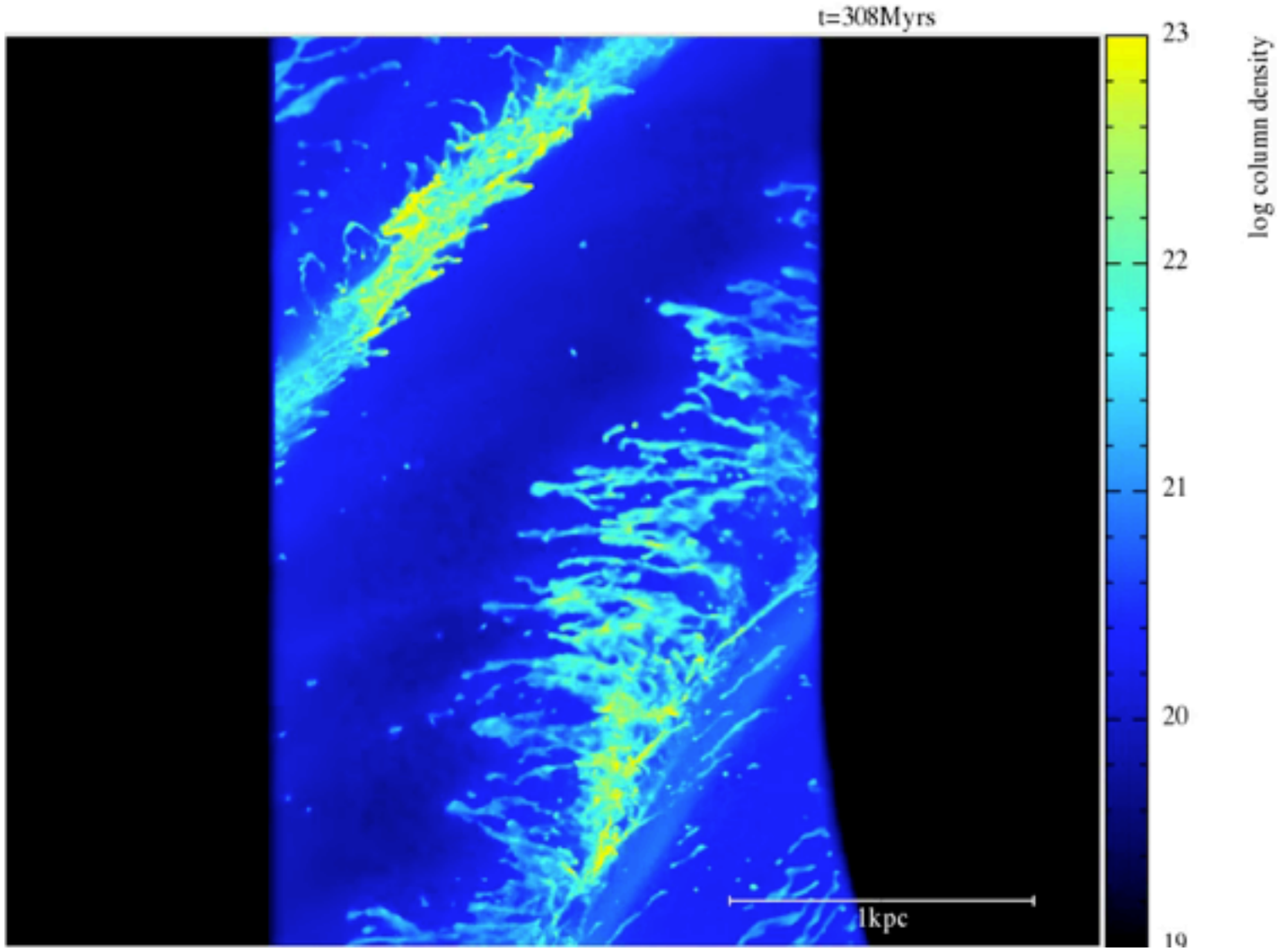
Futur member: L. Majumbdar (3DICE)

+ many collaborators

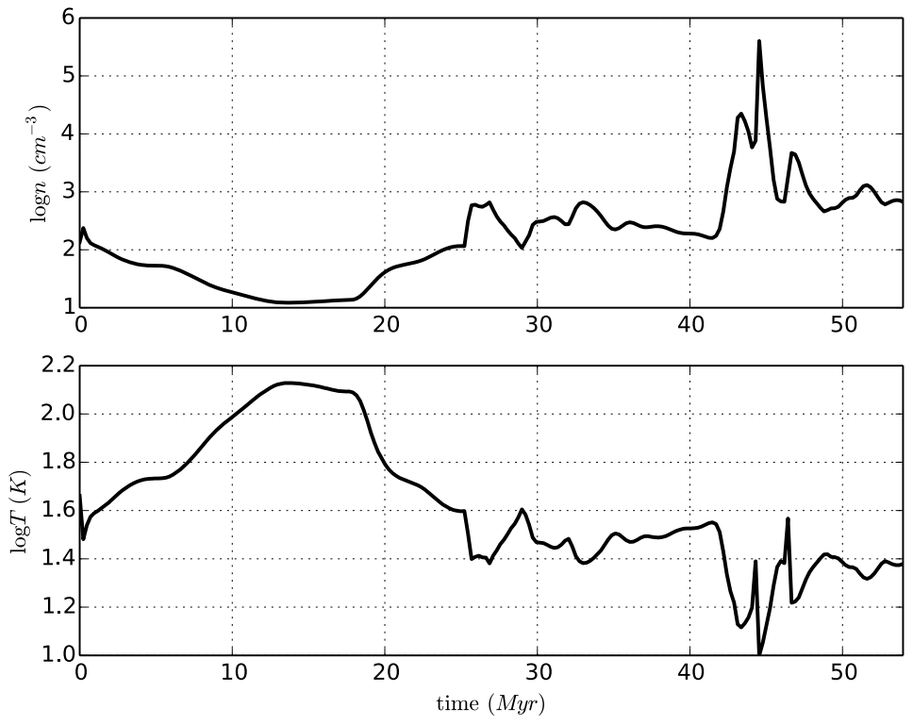


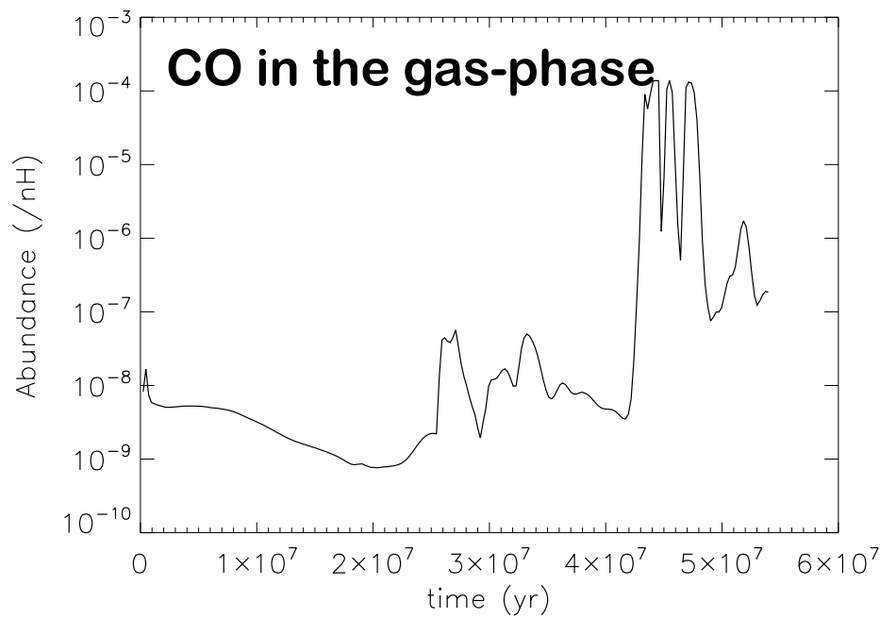
A journey of the interstellar matter

SPH simulations of the ISM at a galactic scale (I. Bonnell et al. 2013)



History of a cell



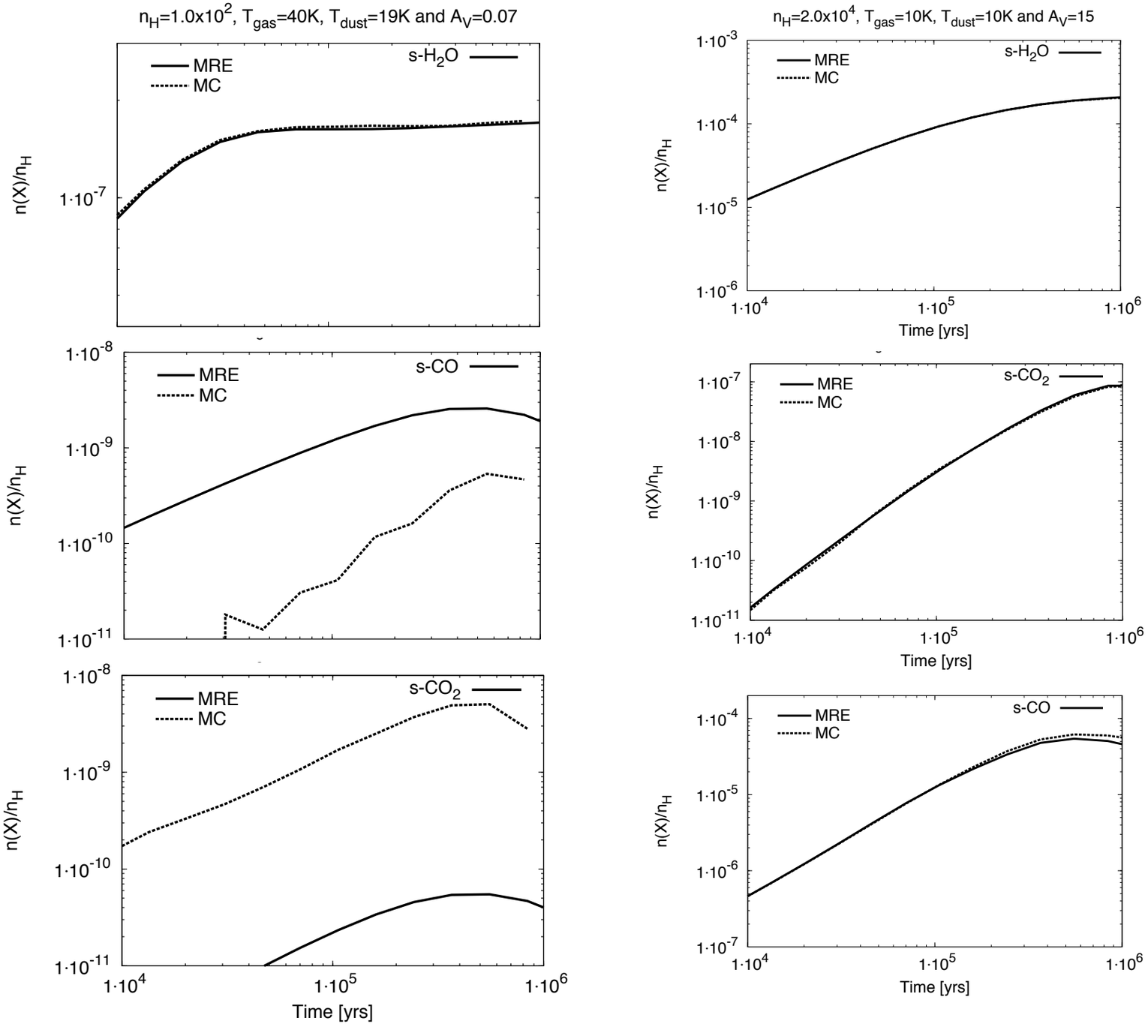


☞ **Work by Pierre Gratier and Maxime Ruaud**

Gas-grain monte-carlo simulations

Nautilus is based on the rate equation approximation not valid at low temperature when they is less than one species on the grains on the grains.

Development of a Monte-Carlo model.

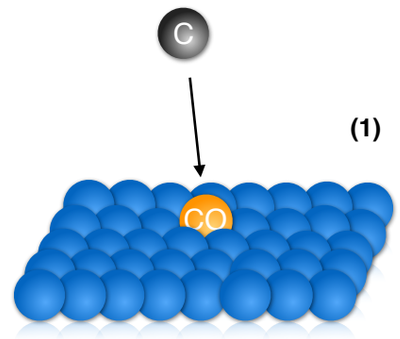


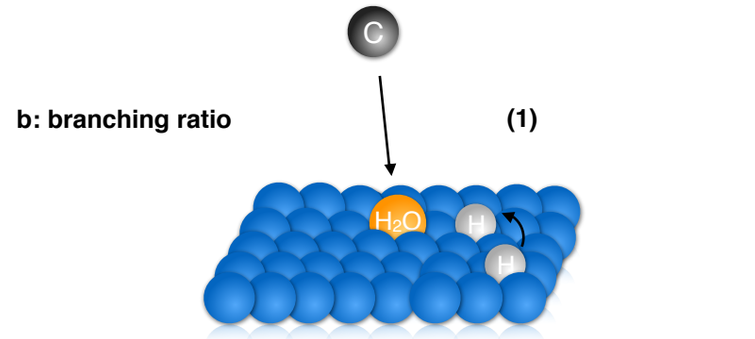
☞ **Work by Maxime Ruaud and Franck Hersant**

New surface chemistry

New surface processes:

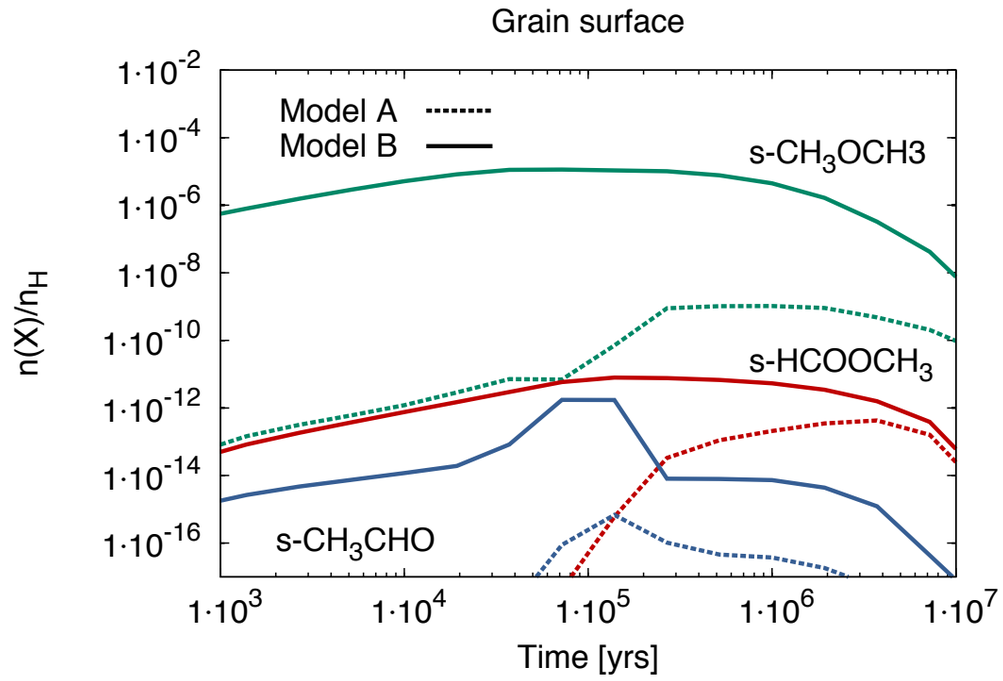
- Low temperature Eley-Rideal (ex: C + s-CO → s-CCO)
- Formation of complexes with the major ice components → different chemistry





Strong influence on some of the surface species including the COMs.
No photodesorption (see also Wakelam et al. 2014).

Model A = old chemistry
Model B = New chemistry



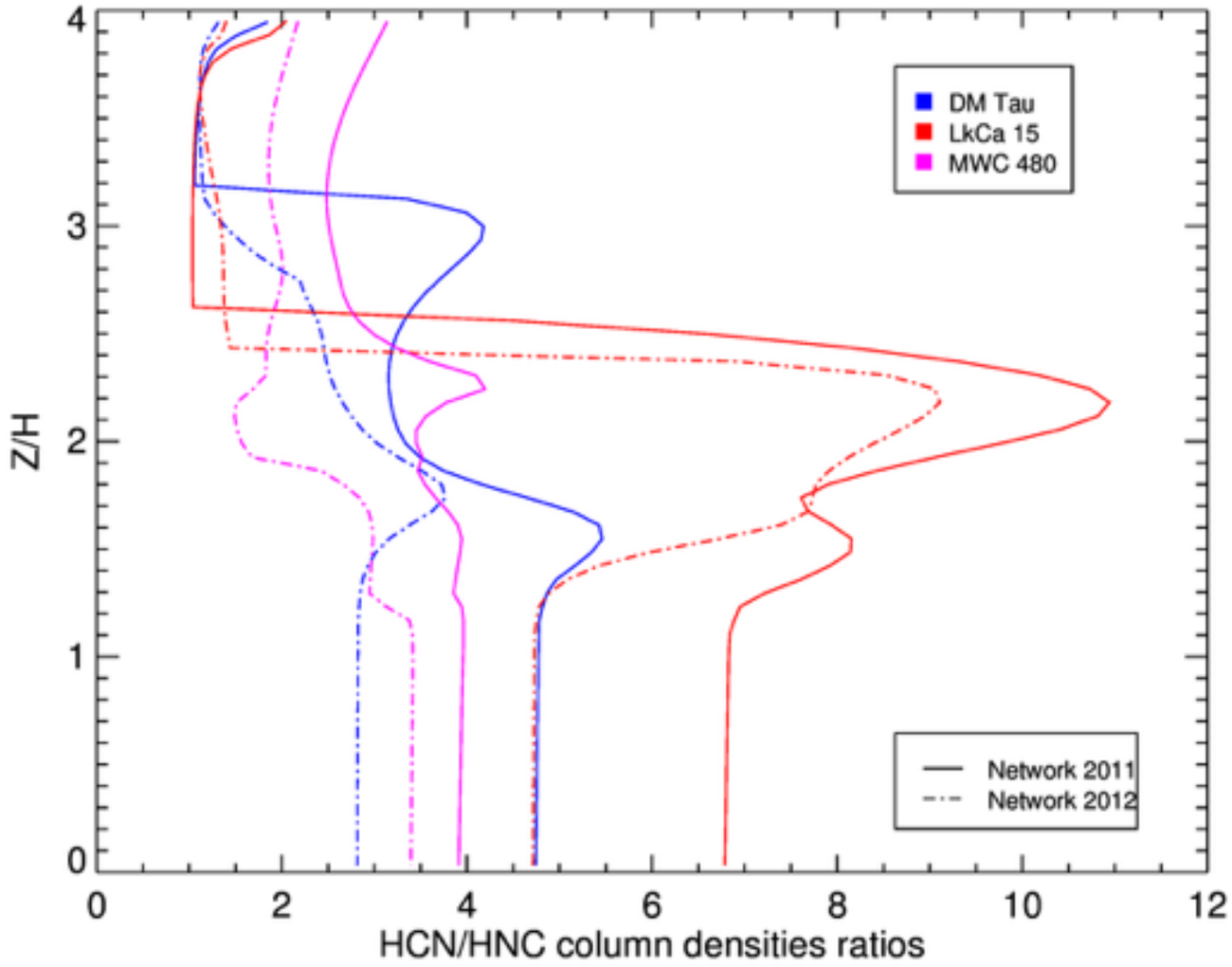
☞ **See Maxime Ruaud's poster**
☞ **Ruaud, Loison et al. (in prep)**

Chemistry in protoplanetary disks

- Improvement of the disk chemistry

- Update of the network from Loison et al. (2014)

- Modeling of HCN and HNC at 300 AU in three disks



☞ See Laura Reboussin's poster
☞ Reboussin et al. (in prep)

Database activities - KIDA

Database of chemical reactions for astrochemistry (interstellar medium and planetary atmospheres)

KIDA
KINETIC DATABASE FOR ASTROCHEMISTRY

- **Engineer working exclusively on KIDA (B. Pavone)**

- **Many recent updates**
- **Possibility to put isotopes into KIDA**

- **Revision of the KIDA logo**
- **Revision of the website**

- **New kida.uva soon available (with its list of references)**
- **Renewing the expert committee**
- **Extension of KIDA to surface reactions**

KIDA | KINETIC DATABASE FOR ASTROCHEMISTRY

Home Models Help References Contact Download Sign in

KIDA is a database of kinetic data of interest for astrochemical (interstellar medium and planetary atmospheres) studies.

C, C+, C + H

SEARCH

Indicate a species (ex: CH, H3O+) or a couple of species (ex: C + H2)
Warning : Second letter of 2-letters elements have to be lowercase, eg Na
Warning : Second letter of 2-letters elements have to be lowercase, eg Na

@kida_database 08:27, Oct 21

RT @ESA_Rosetta Win a trip to @esa #67P landing event by suggesting name for @philae2014 landing site! http://t.co/JI9S641mkV #NameJ

Credits Team

MAILING LIST *Email* SUBSCRIBE UNSUBSCRIBE GO

VAMDC consortium Europlanet erc European Research Council University of Virginia

2014 - Lorem ipsum dolor sit amet, consectetur adipiscing elit.
Donec pretium convallis imperdiet.

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Discussion on the data model

Database activities - KIDA

Communication:

- http://kida.obs.u-bordeaux1.fr/
- News letter
- KIDA on TWITTER (@kida_database)
- The KIDA workshop from May, 5th to 7th 2015 in Paris (http://kida2015.sciencesconf.org)

Statistics:

Sessions	Utilisateurs	Taux de rebond	% nouvelles sessions
5 052	1 947	15,08 %	36,30 %

Pays/Territoire	Acquisition			Comportement
	Sessions	% nouvelles sessions	Nouveaux utilisateurs	Taux de rebond
	5 052 % du total: 100,00 % (5 052)	36,36 % Moyenne du site: 36,30 % (0,16 %)	1 837 % du total: 100,16 % (1 834)	15,08 % Moyenne du site: 15,08 % (0,00 %)
1. France	2 234 (44,22 %)	22,92 %	512 (27,87 %)	12,00 %
2. United States	646 (12,79 %)	50,15 %	324 (17,64 %)	11,30 %
3. Germany	323 (6,39 %)	49,23 %	159 (8,66 %)	9,29 %
4. Japan	187 (3,70 %)	40,11 %	75 (4,08 %)	17,11 %
5. Netherlands	178 (3,52 %)	42,13 %	75 (4,08 %)	12,36 %
6. Sweden	175 (3,46 %)	8,57 %	15 (0,82 %)	52,57 %
7. United Kingdom	149 (2,95 %)	47,65 %	71 (3,86 %)	11,41 %
8. Italy	147 (2,91 %)	31,97 %	47 (2,56 %)	30,61 %
9. Spain	91 (1,80 %)	52,75 %	48 (2,61 %)	10,99 %
10. Czech Republic	85 (1,68 %)	28,24 %	24 (1,31 %)	9,41 %

~200 registered users

Database activities - KIDA

Models

File	Comment	Added on
reboussin2014.zip	Type of chemistry : Gas-phase and gas-grains Number of reactions : 9127 Number of species : 703 Publication : Reboussin et al. 2014, MNRAS, 440, 3557 Description : Gas-phase and gas-grains chemical network for dense interstellar medium. The gas-phase has been updated compared to kida.uva.2011, using reactions of carbon chains and nitrogen chains proposed by Loison et al. (2014a,b). The surface network has been modified to include new CRID process.	2014-09-15 13:08:47
Nahoon_public_aug2013_web_unc.zip	Update version of the Nahoon chemical model. Bug fixed on the temperature dependence in case of duplicated reactions with complementary ranges of temperature.	2013-09-04 10:23:13
Hincelin2013.tar.gz	Type of chemistry: Gas-grains Publication: Hincelin et al. 2013, ApJ, in press Description: Format of the network is described in a readme file.	2013-07-26 21:03:23
Chabot2013.zip	Type of chemistry: Gas-phase Number of reactions: Number of species: Publication: Chabot et al. 2013, ApJ, 771, id 90 Description: Two different gas-phase networks are available: one for dense clouds with a format similar to kida.uva.2011 and one for PdR regions with a format similar to the Meudon PDR code (format described at http://pdr.obspm.fr/PDRcode_Chemistry.html). Both networks have been updated according to the suggestions made in the paper.	2013-06-28 10:07:08
osu_highT.zip	Type of chemistry: Gas-phase Number of reactions: 5387 Number of species: 461 Publication: Harada, Herbst & Wakelam 2010, ApJ, 721,1570 and Harada, Herbst & Wakelam 2012, ApJ, 756, id. 104 Description: Gas-phase network for temperatures up to 800 K.	2012-10-05 10:05:10
nls_react_kida_2010_druard.dat.zip	Type of chemistry: Gas-grain Number of reactions: 6215 Number of species: 666 Publication: Druard & Wakelam 2012, MNRAS 426, 354-359 (http://arxiv.org/abs/1207.5325) Description: Network modified in order to include new reactions for polysulfanes, sulphur polymers and CS2.	2012-07-26 14:38:47
PAHs.zip	List of reactions involving PAHs used in Wakelam & Herbst (2008). The format of the network is the same as the OSU database. Some details are given in a pdf file.	2012-06-27 14:15:56
Nahoon_public_oct2011_web_unc.zip	New version of the Nahoon chemical model. See the newly accepted paper by Wakelam et al. (ApJS) for a full description: http://kida.obe.u-bordeaux1.fr/uploads/documents/kida_apj.pdf	2012-01-27 15:13:54
kida.uva.2011.zip	New gas-phase chemical network for dense interstellar medium called kida.uva.2011. This is a new version of the OSU database updated according to the latest recommendations from the KIDA experts until October 2011. The network is described in a paper accepted for publication by ApJS (download here: http://kida.obe.u-bordeaux1.fr/uploads/documents/	2012-01-27 15:11:12
astrochem.html	Astrochem is a code to study the chemistry of a va gas-grain interactions, such as depletion and deso between hundreds of species can be solved in a fe Sébastien Maret.	

~400 downloads per year

File	Comment	Added on
Chemistry_review_S_Titan.pdf	Type of chemistry: Neutral-neutral gas-phase reactions. Publication: The evolution of infalling sulfur species in Titan's atmosphere, Hickson et al 2014, A&A Description: This chemical network was constructed to model sulfur chemsitry for Titan.	2014-09-24 15:00:19
Hebrard2013.zip	Type of chemistry: Neutral-neutral gas-phase reactions Number of reactions: 941 Number of species: 90 Publication: Hébrard et al., 2013 Hébrard et al., 2013 - Astron. Astrophys. (DOI: 10.1051/0004-6361/201220686) Description: This updated chemical network was constructed to model C3 hydrocarbon chemistry in Titan's atmosphere. See the paper for more details. Please refer to the README file included in the .zip file for the reading format.	2013-07-26 21:05:45
Venot2012.zip	Type of chemistry: C/H/O/N neutral-neutral gas-phase reactions Number of reactions: 957+6 Number of species: 105 Publication: Venot et al., 2012, A&A 546, id.A43 (DOI 10.1051/0004-6361/201219310) Description: Gas-phase chemical network for modeling the kinetic evolution of radicals and molecules containing less than three carbon atoms in the atmospheres of hot Jupiters. Please refer to the README file included in the .zip file for the reading format.	2012-07-05 09:57:36
Hebrard2012.zip	Type of chemistry: Neutral-neutral gas-phase reactions Number of reactions: 788 Number of species: 86 Publication: Hébrard et al., 2012 - Astron. Astrophys. (DOI: 10.1051/0004-6361/201218837) Description: This updated chemical network was constructed to model HCN and HNC chemistry in Titan's atmosphere. See the paper for more details. Please refer to the README file included in the .zip file for the reading format.	2012-05-11 10:04:26

KIDA

KINETIC
DATABASE
FOR
ASTROCHEMISTRY

UNIVERSITY of VIRGINIA

VAMDC consortium

Funding:

erc European Research Council

ASTRONET

SEVENTH FRAMEWORK PROGRAMME

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