Structuration
Données Atomiques and Moléculaires

M.L. Dubernet
LERMA, Paris Observatory
10/04/2006

Collaborations:
E. Roueff (LUTH, Obs. Paris), P. Osuna & M. Guanazzi (ESAC, Spain),
Y. Ralchenko (NIST), B. Clarck (IAEA), D. Schultz (Oackridge)
S.Derrière (CDS for UCD)

MLD acknowledges support from MDA project, VO-France, Paris Observatory

Motivation

- Scientific Use cases
  - ** Identification of lines in observed spectra (ISO, Herschel, Alma, Spitzer, etc...) : spectroscopic data
  - ** Analysis of spectra for non-ETL media : spectroscopic+collisional data
  - ** Simulation of Interstellar Medium, circumstellar/planetary/cometary atmospheres : models + spectroscopic data + chemistry (collision, reaction, etc..)
  - ** etc ..

Project Overview (1)

- **Access Atomic/Molecular DB starting with line lists**
  - **Theoretical (measured or calculated) DB**
  - **Observed line lists DB**
- **Necessary to access complementary information in order to interpret spectra or model astrophysical media: excitation rate coefficients, etc..**
- **Clients: stronger evolution towards public software packages for spectral analysis and on line codes for astro. Simulation**
  - Shared, structured, complete and documented access to AM DB
  - Standardisation O/I, queries, ressources ID

Overview (2)

- **Numerous DB are available**
  - Atomic lines: NIST DBs, Kurucz's CD-ROM, Atomic Line List of P. Van Hoof, TOPbase, Kelly Atomic Line DB, VALD, MCHF/MCDHF Collection, D.R.E.A.M, KAERI AMODS
  - Molecular Lines: JPL Spectroscopic DB, CDMS, HITRAN, GEISA, NIST
  - Other DB: IEAE, NIFS, CHIANTI, UMIST, BASECOL, small compilations
  - Observed databases: ATOMDB, NIST, ...
- **Identification of Pbs**
  - Different DB have similar datasets
    - DB have different levels of update
    - Lengthy to identify origin of datasets, find all relevant description of data
  - Useful data for a single astrophysical application are dispersed in various DB
    - No homogeneous description of data

Global Structure

- Identification of Chemical Elements
- Identification of levels
- Radiative transitions between bound states
- Photon-Matter Interaction
- Matter-Matter Interaction
  - Processes: ionization, reaction, ...
  - Observables: cross-sections, rate coefficients, etc...

Led to a list of UCD

« Atomic and Molecular UCD », M.L. Dubernet & E. Roueff, May 2004 – Preliminary document to final UCD list kept by CDS/IVOA

DM : general transition model

Matter – Matter Interaction

Excitation : A(i) + B(k) --> A(j) + B(l)

- TargetLine = Line : A
  - initialElement=finalElement
  - InitialLevel = i ; finalLevel = j
- PerturberLine = Line : B
- Other attributes specific to excitation
  - Temperature
  - Rate coefficients

Reaction : AB(i) + C(k) --> A(j) +BC(l)

- Reactant = (1 to *) Line: AB, C
  - InitialChemical: AB or C
    - InitialLevel_species : i
    - FinalLevel_species : none
  - FinalChemical: none
- Products = (1 to *) Line: A, BC
    - Reverse identification

Spectral Line Access Protocol

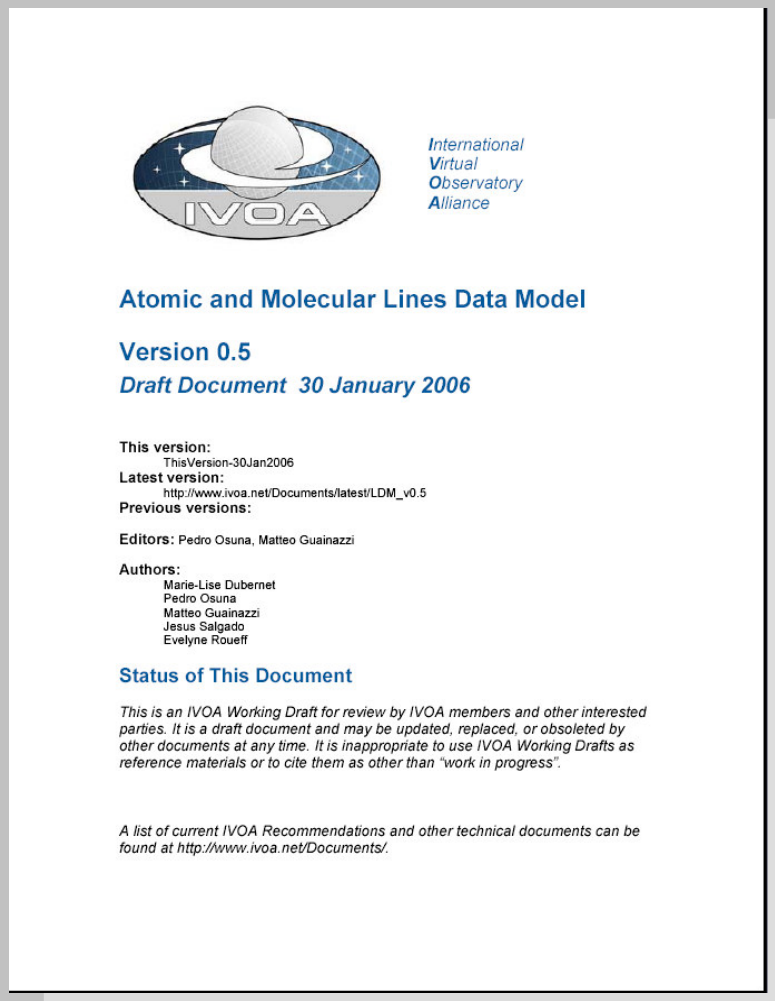
Paris Observatory and ESA/ESAC

ML Dubernet, P. Osuna, M. Guanazzi,

J. Salgado, E. Roueff

MLD acknowledges support from VO-France, MDA project,
Paris Observatory

Documents status and perspectives



International
Virtual
Observatory
Alliance

Atomic and Molecular Lines Data Model

Version 0.5

Draft Document 30 January 2006

This version:
ThisVersion-30Jan2006
Latest version:
http://www.ivoa.net/Documents/latest/LDM_v0.5
Previous versions:

Editors: Pedro Osuna, Matteo Guainazzi

Authors:
Marie-Lise Dubernet
Pedro Osuna
Matteo Guainazzi
Jesus Salgado
Evelyne Roueff

Status of This Document

This is an IVOA Working Draft for review by IVOA members and other interested parties. It is a draft document and may be updated, replaced, or obsoleted by other documents at any time. It is inappropriate to use IVOA Working Drafts as reference materials or to cite them as other than "work in progress".

A list of current IVOA Recommendations and other technical documents can be found at http://www.ivoa.net/Documents/.

- *AML DM Current version*: 0.5 (30/1/2006)
- SLAP *Current version*: 0.1

- circulated to the DM and DAL groups, as well as to atomic and molecular astrophysicists for comments

- *Ultimate goal:* achieve the status of a *proposed recommendation* by the **next InterOp meeting for AML DM**

- **Useful for LTE studies and calibration**

Access to Lines: DataModel

- Based on fundamental physics, current databases and needs in astrophysics
- Current DM is centered around line for atom and molecules: electronic, vibrational, rotational transitions (couplings)
- Allows for identification of
  - Chemical Species
  - Level -->Quantum State-->Quantum numbers
  - Origin and modification of Line (Observed lines)
- Some parts could be re-used to model other processes involving transitions because a line corresponds to a transition between two levels

DM : general transition model

- Each time a species undergoes a transition, it can be modeled by a Line DM

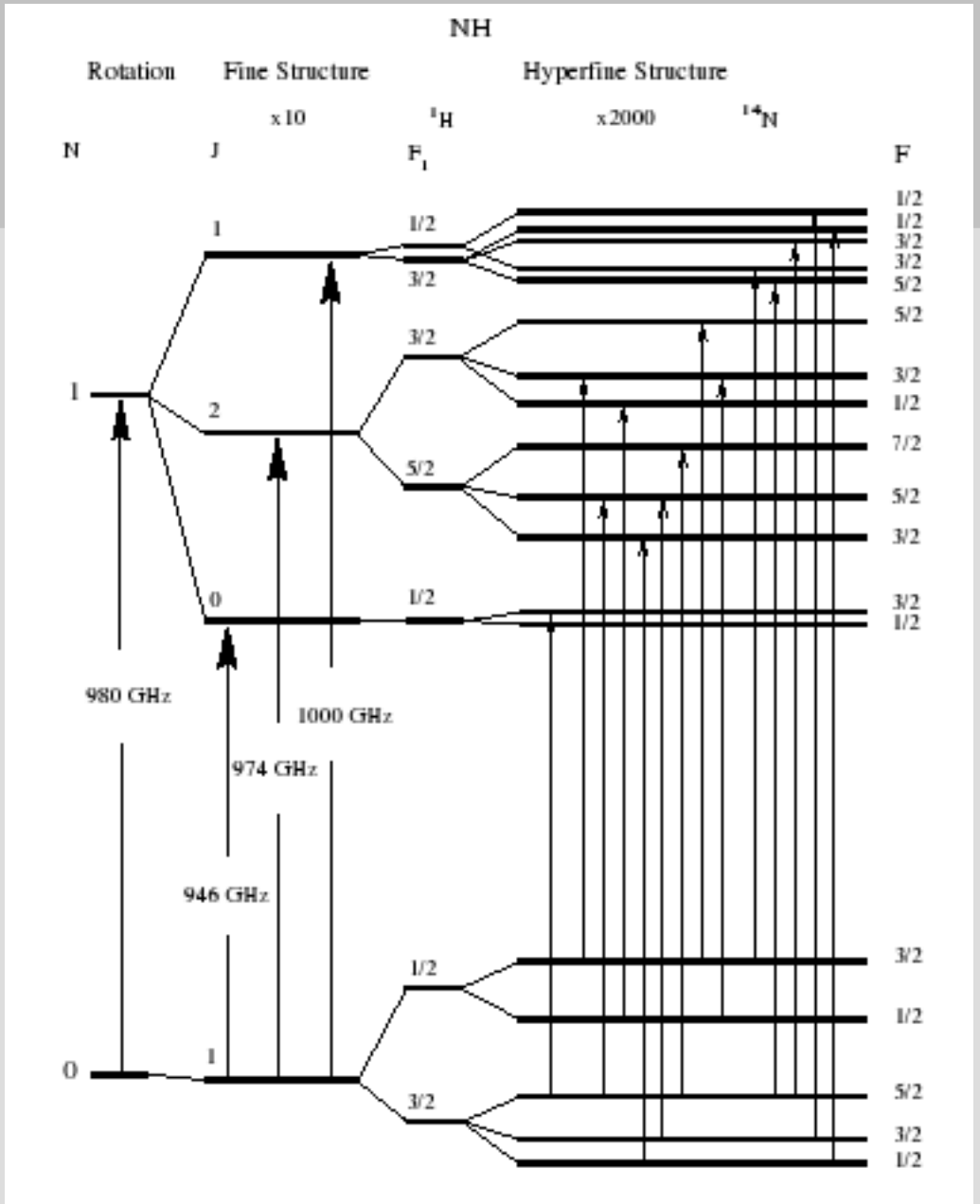
A transition is modeled by

Before .... Oups Something happens! ... After

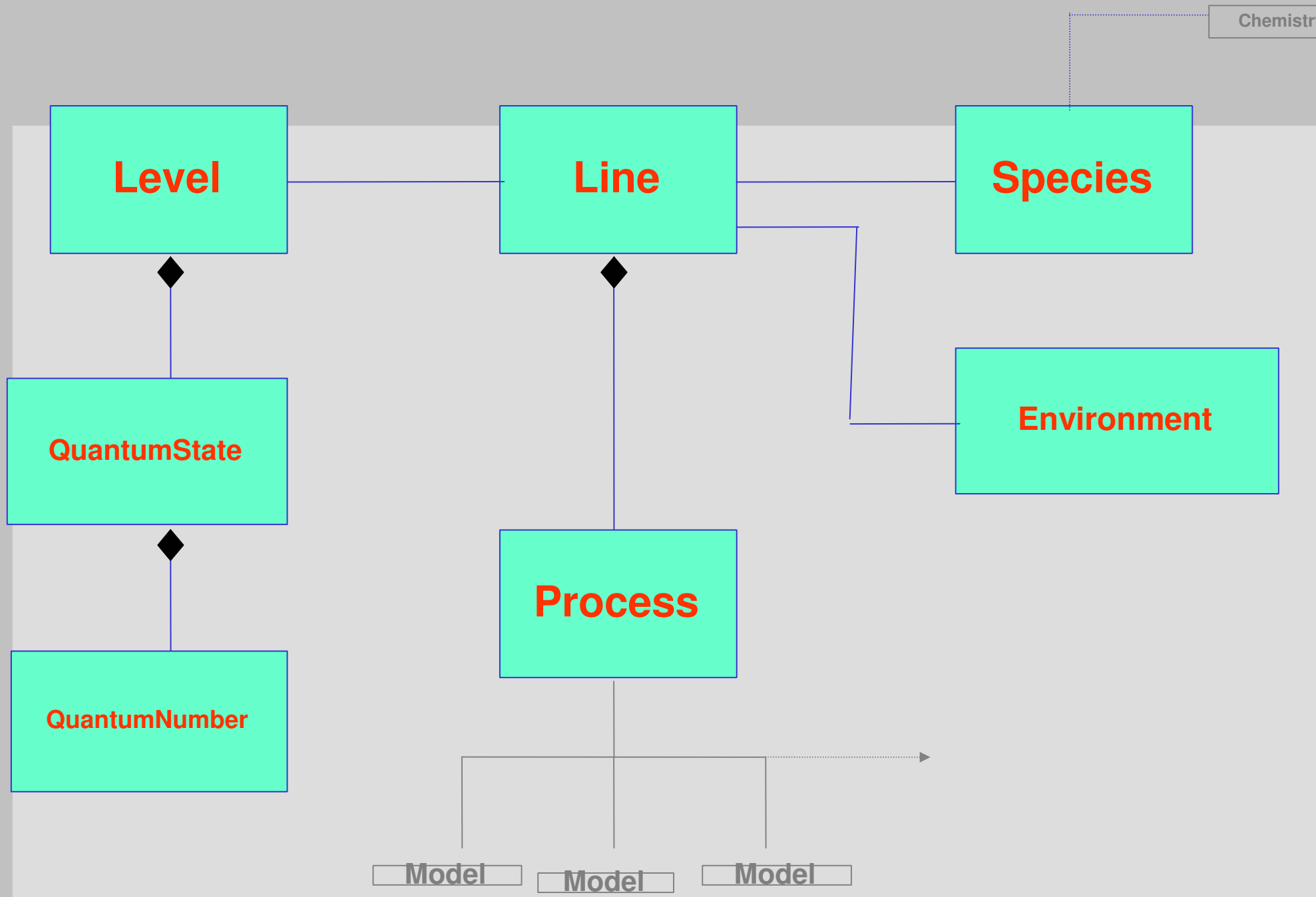
Light – Matter Interaction : bound-bound

$$A(j) + hv \dashrightarrow A(j')$$

$$A(j') \dashrightarrow A(j) + hv$$


NH
Rotation
Fine Structure
x10
^{1}H
Hyperfine Structure
x2000
^{14}N
N
J
F_1
F
1
2
0
1
1/2
3/2
5/2
7/2
980 GHz
1000 GHz
974 GHz
946 GHz

Structure


Chemistry
Level
Line
Species
QuantumState
Environment
Process
QuantumNumber
Model
Model
Model

Line

- Scope: describe the overall properties of the observed line, and of its corresponding transition

Attributes:

- Observational properties:
  - wavelength
  - intensity/flux
  - significance
  - broadening
  - wavelength shift
- Transition properties:
  - Einstein coefficients
  - oscillator strengths
  - transition type

Level – QuantumState - QuantumNumber

Scope: describe the quantum state of the levels, between which the transition originating the line occurs

- Attributes:
  - Level:
    - energy (with its origin) and configuration
    - statistical weight
    - lifetime
    - quantum constants (Lande factor etc.)
    - Parity, symmetries
  - Quantum state:
    - normalized probability
    - term symbol
    - quantum numbers

Quantum Number: coupling

- N_2H^+ : rotationN, 2 nuclearSpinI for Nitrogen
- level characterized with a single state $|NF_1F>$
- $N+I_1= F_1$; $F_1+I_2=F$
- QuantumNumber : F

  label = F

  type = totalAngularMomentumF

  origin1 = F_1

  origin2 = I_2

  numeratorValue = 1

  denominatorValue = 1

  description = « resulting total angular momentum; coupling of I_2 and F_1

DM : general transition model
Light-Matter : bound-continuum

- Radiative recombinaison

(Z, N-1)[level.of.Z(N-1)] + e ---> (Z, N)[level.of.Z(N)] + hv

InitialElement = ChemicalElement

IonizationStage = -1 (comparatively to N)

Z is specified

full atomic symbol is specified (see DM)

FinalElement = ChemicalElement

IonizationStage = 0 (comparatively to N)

Z is specified

full atomic symbol is specified (see DM)

DM : missing Provenance

- Observations : see characterization
- Measured Data : instrument and parameters
- Calculated sets : VOTheory
  - Various steps in getting final data, ex :
    - Method
      - Hamiltonian (parameters, approximations), basis sets
    - Algorithms
  - Fitting functions: parameters, function, error
  - Etc...

DAL: Query Parameters

- **SLAP : Simple Line Access Protocol**
  - By wavelength_min, _max, _mid
  - By species: Fe I, H_20, ...
  - By type of transition (E1, M1, E2)
  - By type of levels (vibration, rotation, ..)
  - Combined with associated processes

Access to Lines: SLAP

- What information do we retrieve from a service implementing SLAP?
  - Wavelength : mandatory
  - Initial/Final ChemicalElement : should
    - Name or atomicSymbol/formula : should
  - Initial/Final Level : should
    - QuantumState : should
    - energy, statWeight : should
  - Einstein A : should
  - Optional : everything else

Note on UCD/utype

- UCD seem heavy and too vague to be used efficiently for exchange of atomic and molecular data
- UCD might be useful to « globally » search datasets if tools are developped
- Utype seems more useful for now

Contacted people

Physicists, Databases, Astronomers

- GEISA: N. Husson-Jacquinet
- HITRAN: L. Rothman
- CDMS: S. Schlemmer
- JPL: J. Pearson
- UMIST: T. Millar
- CHIANTI: P. Young
- DREAM: P. Quinet
- TOPBase: C. Zeippen
- NIST: F. Lovas, Y. Ralchenko
- NIFS: T. Kato
- IEAE: B. Clark
- KAERI: Y.-J. Rhee
- ATOMDB: N. Brickhouse
- D. Schwenke
- J. Tennyson
- A bunch of french spectroscopists
- J. Aboudarham (solar)
- B. Plez (stars)
- J. Cernicharo (ISM)
- F. Valdes (calibration package)

Application: Basecol Database

http://www.obspm.fr/basecol

ML Dubernet
LERMA, Paris Observatory

Present Engineer: N. Moreau*
Present Contributors: M.L. Dubernet*, F. Daniel*, D. Flower***, A. Grosjean**
Past Contributors: B. Debray**, G. Souemes*

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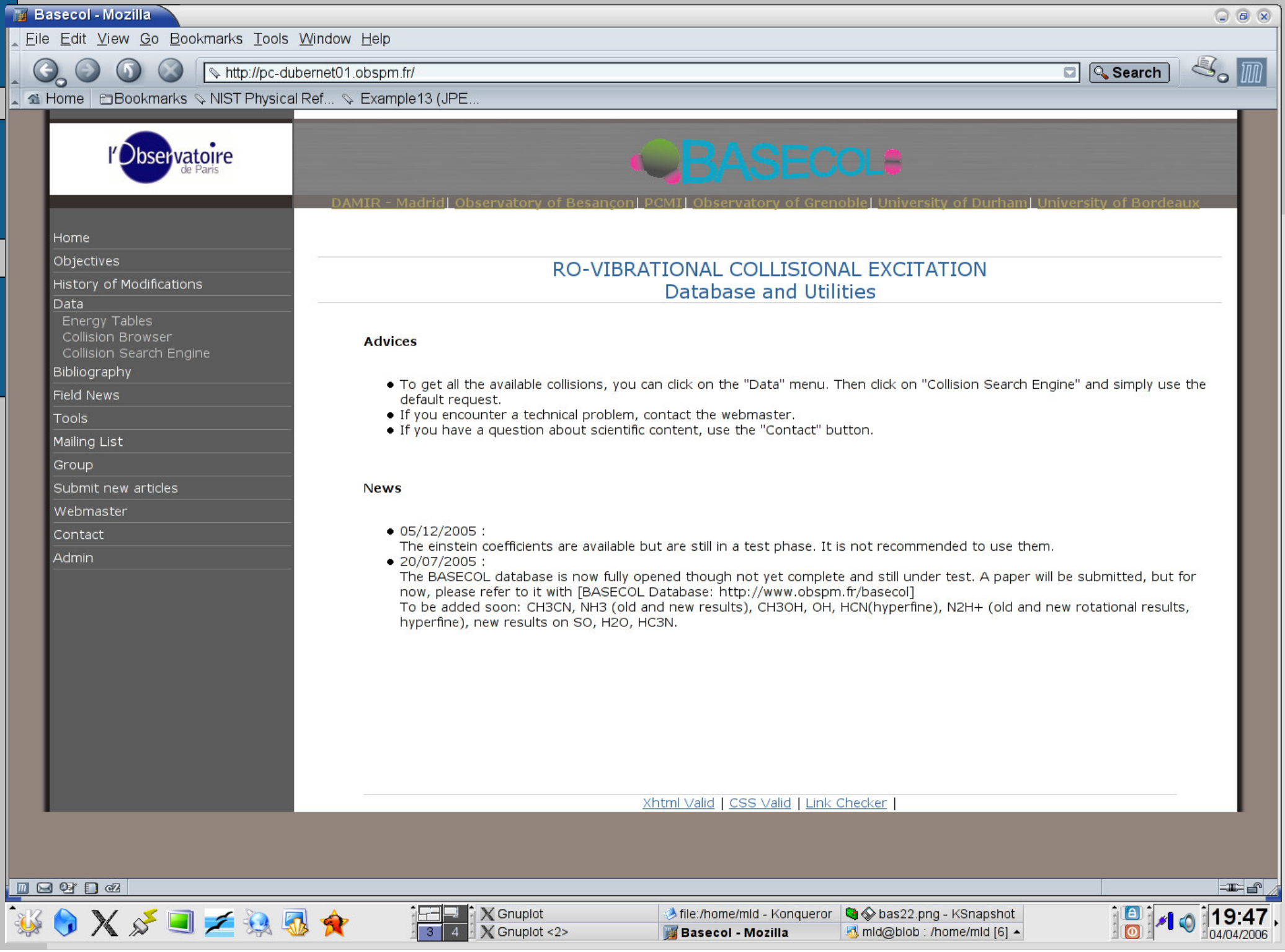
* *LERMA, Paris Observatory*
** *Besançon Observatory*
*** *Durham University, UK*

Objectives/Content

- Useful for astrophysicists and physicists
- Published (de)-excitation rate coefficients
  - Rotational (fine, hyperfine structure)
  - Ro-vibrational, Vibrational (not exhaustive)
  - Currently: 21 Target molecules
  - Perturbers : He, H, H_2 (not exhaustive)
  - 76 collisional systems
- Fully documented and referenced (630 ref.)
- Linked to
  - Theoretical energy levels
  - Experimental energy levels, Einstein coefficients(CDMS or JPL)
- Fitting coefficients, visualisation tools


Basecol - Mozilla
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http://pc-dubernet01.obspm.fr/
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Home Bookmarks NIST Physical Ref... Example13 (JPE...
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RO-VIBRATIONAL COLLISIONAL EXCITATION
Database and Utilities
Advices
To get all the available collisions, you can click on the "Data" menu. Then click on "Collision Search Engine" and simply use the default request.
If you encounter a technical problem, contact the webmaster.
If you have a question about scientific content, use the "Contact" button.
News
05/12/2005 :
The einstein coefficients are available but are still in a test phase. It is not recommended to use them.
20/07/2005 :
The BASECOL database is now fully opened though not yet complete and still under test. A paper will be submitted, but for now, please refer to it with [BASECOL Database: http://www.obspm.fr/basecol]
To be added soon: CH3CN, NH3 (old and new results), CH3OH, OH, HCN(hyperfine), N2H+ (old and new rotational results, hyperfine), new results on SO, H2O, HC3N.
Xhtml Valid | CSS Valid | Link Checker |
Gnuplot
Gnuplot <2>
file:/home/mld - Konqueror
Basecol - Mozilla
bas22.png - KSnapshot
mld@blob : /home/mld [6]
19:47
04/04/2006

Basecol - Mozilla

File Edit View Go Bookmarks Tools Window Help

http://pc-dubernet01.obspm.fr/index.php?pag

Home | Bookmarks | NIST Physical Ref... | Example13 (JPE...

l'Observatoire de Paris

DAMIR - Madrid | Observat

- Home
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- Data
  - Energy Tables
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  - Collision Search Engine
- Bibliography
- Field News
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- Submit new articles
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- Contact
- Admin

<< Back to collision's details

CO initial levels : 1-3

H2 initial levels : 1-1

CO final levels : 1-3

H2 final levels : 1-1

Temperatures : 5-4

Enter numbers (separated by ';') or/and an interval (with '-')
Example : 1;9-21;23

1 : CO
2 : H2

Mozilla

File Edit View Go Bookmarks Tools Window Help

http://pc-dubernet01.obspm.fr/match/34_Einstein_CDMS_2006-02-14.txt

Home | Bookmarks | NIST Physical Ref... | Example13 (JPE...

number of lines : 29

Initial level	Final level	Frequency	Einstein coefficient	Log(A)	Uncertainty
2	1	115271.2018	7.2034148e-8	-7.1425	0.0005
3	2	230538.0000	6.9103080e-7	-6.1605	0.0005
4	3	345795.9899	2.4965589e-6	-5.6027	0.0005
5	4	461040.7682	6.1263650e-6	-5.2128	0.0005
6	5	576267.9305	1.2212740e-5	-4.9132	0.0005
7	6	691473.0763	2.1374069e-5	-4.6701	0.0005
8	7	806651.8060	3.4222452e-5	-4.4657	0.0050
9	8	921799.7000	5.1339745e-5	-4.2895	0.0050
10	9	1036912.3930	7.3298304e-5	-4.1349	0.0050
11	10	1151985.4520	1.0063605e-4	-3.9972	0.0110
12	11	1267014.4860	1.3390036e-4	-3.8732	0.0050
13	12	1381995.1050	1.7353034e-4	-3.7606	0.0130
14	13	1496922.9090	2.2003922e-4	-3.6575	0.0120
15	14	1611793.5180	2.7390517e-4	-3.5624	0.0110
16	15	1726602.5057	3.3536041e-4	-3.4745	0.0024
17	16	1841345.5060	4.0500226e-4	-3.3925	0.0110
18	17	1956018.1390	4.8289379e-4	-3.3161	0.0110
19	18	2070615.9930	5.6952029e-4	-3.2445	0.0140
20	19	2185134.6800	6.6502238e-4	-3.1772	0.0130
21	20	2299569.8420	7.6955157e-4	-3.1138	0.0100
22	21	2413917.1130	8.8331834e-4	-3.0539	0.0110
23	22	2528172.0600	1.0064098e-3	-2.9972	0.0110
24	23	2642330.3459	1.1389669e-3	-2.9435	0.0039
25	24	2756387.5840	1.2806260e-3	-2.8926	0.0170
26	25	2870339.4070	1.4318806e-3	-2.8441	0.0130
27	26	2984181.4550	1.5920620e-3	-2.7980	0.0140
28	27	3097909.3610	1.7614786e-3	-2.7541	0.0170
29	28	3211518.7506	1.9397870e-3	-2.7122	0.0047
30	29	3325005.2827	2.1265850e-3	-2.6723	0.0051

Label	Energy	N	v1
1	0.0000	0	0
2	3.8450	1	0
3	11.5350	2	0
4	23.0695	3	0
5	38.4481	4	0
6	57.6704	5	0
7	80.7354	6	0
8	107.6424	7	0
9	138.3904	8	0
10	172.9780	9	0
11	211.4041	10	0
12	253.6672	11	0
13	299.7656	12	0
14	349.6975	13	0
15	403.4612	14	0
16	461.0545	15	0
17	522.4751	16	0
18	587.7209	17	0
19	656.7892	18	0
20	729.6774	19	0
21	806.3828	20	0
22	886.9024	21	0
23	971.2332	22	0
24	1059.3718	23	0
25	1151.3150	24	0
26	1247.0592	25	0
27	1346.6008	26	0
28	1449.9360	27	0
29	1557.0607	28	0
30	1667.9709	29	0

I1	F1	I2	F2	5	10	20	30	40	50	60	70	80
1	1	1	1	+3.55e-09	+2.72e-09	+2.02e-09	+1.9e-09	+1.94e-09	+2.02e-09	+2.13e-09	+2.19e-09	+2.28e-09
1	2	1	1	+2.53e-11	+4.85e-11	+6.45e-11	+7.48e-11	+7.98e-11	+8.4e-11	+8.86e-11	+9.32e-11	+9.62e-11
1	3	1	1	+3.82e-12	+2.17e-11	+5.54e-11	+7.73e-11	+9.4e-11	+1.04e-10	+1.14e-10	+1.18e-10	+1.26e-10
1	4	1	1	+5.84e-14	+1.63e-12	+8.89e-12	+1.65e-11	+2.39e-11	+3.06e-11	+3.74e-11	+4.29e-11	+4.9e-11
1	5	1	1	+2.67e-16	+7.21e-14	+1.3e-12	+3.64e-12	+6.34e-12	+9.09e-12	+1.18e-11	+1.42e-11	+1.67e-11
1	6	1	1	+3.99e-19	+1.83e-15	+1.4e-13	+6.74e-13	+1.62e-12	+2.96e-12	+4.62e-12	+6.58e-12	+8.8e-12
1	7	1	1	+1.72e-22	+2.15e-17	+8.39e-15	+6.87e-14	+2.14e-13	+4.51e-13	+7.71e-13	+1.16e-12	+1.61e-12
1	8	1	1	+1.44e-26	+1.21e-19	+4.11e-16	+7.31e-15	+3.58e-14	+1.04e-13	+2.29e-13	+4.26e-13	+7.06e-13
1	9	1	1	+2.58e-30	+1.18e-21	+2.9e-17	+9.49e-16	+5.96e-15	+1.94e-14	+4.53e-14	+8.69e-14	+1.47e-13
1	10	1	1	+3.39e-35	+2.54e-24	+7.97e-19	+6.22e-17	+6.31e-16	+2.88e-15	+8.75e-15	+2.09e-14	+4.26e-14
1	11	1	1	+6.6e-40	+1.17e-26	+5.18e-20	+9.39e-18	+1.39e-16	+7.52e-16	+2.47e-15	+6.1e-15	+1.25e-14
1	12	1	1	+1.4e-45	+9.01e-30	+8.99e-22	+4.63e-19	+1.16e-17	+8.78e-17	+3.69e-16	+1.11e-15	+2.7e-15
1	13	1	1	+0e+00	+1.19e-32	+3.65e-23	+5.49e-20	+2.28e-18	+2.28e-17	+1.12e-16	+3.7e-16	+9.45e-16

Done

Gnuplot | file:/home/mld - Konqueror | mld@blob : /home/mld [6] | Basecol - Mozilla | Ksnapshot [3]

19:49

Basecol Web Service

- Query for a single molecule
  - Query for a process
  - Query for a collider
  - Query for a temperature range
- Get
  - Rate coefficients
  - Theoretical and experimental energy levels
  - Einstein coefficients and statistical weights
  - Errors
  - Fits
  - Documentation

Link to PDR Numerical Code

Get collisions only

- Query Parameters
  - TARGET, COLLIDER
  - initial_level, final_level
- Return VOTable with
  - List of collisions with TARGET + COLLIDER
  - Link to energy tables (basecol)
  - Link to fitting coefficients

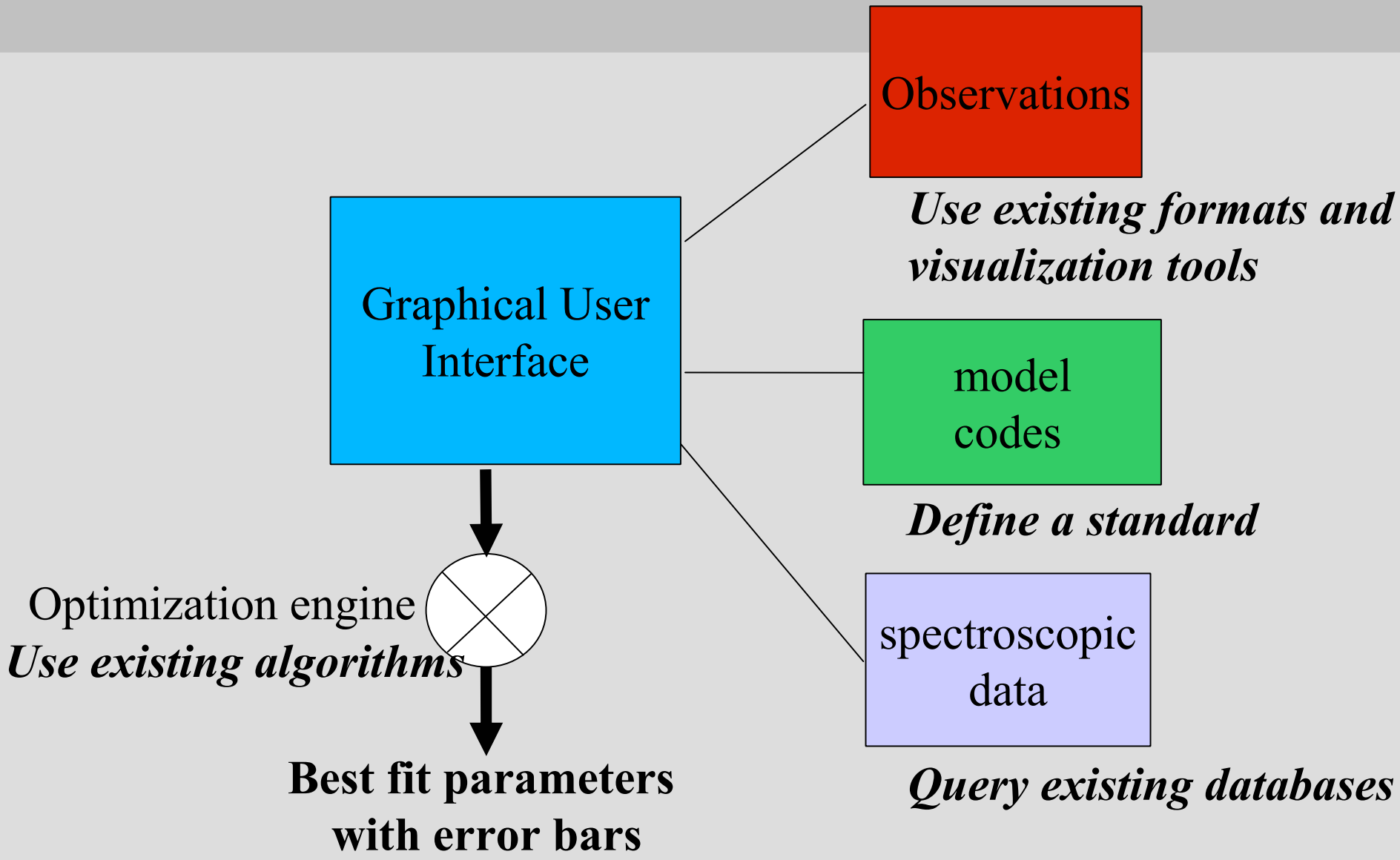
Get CDMS/JPL data

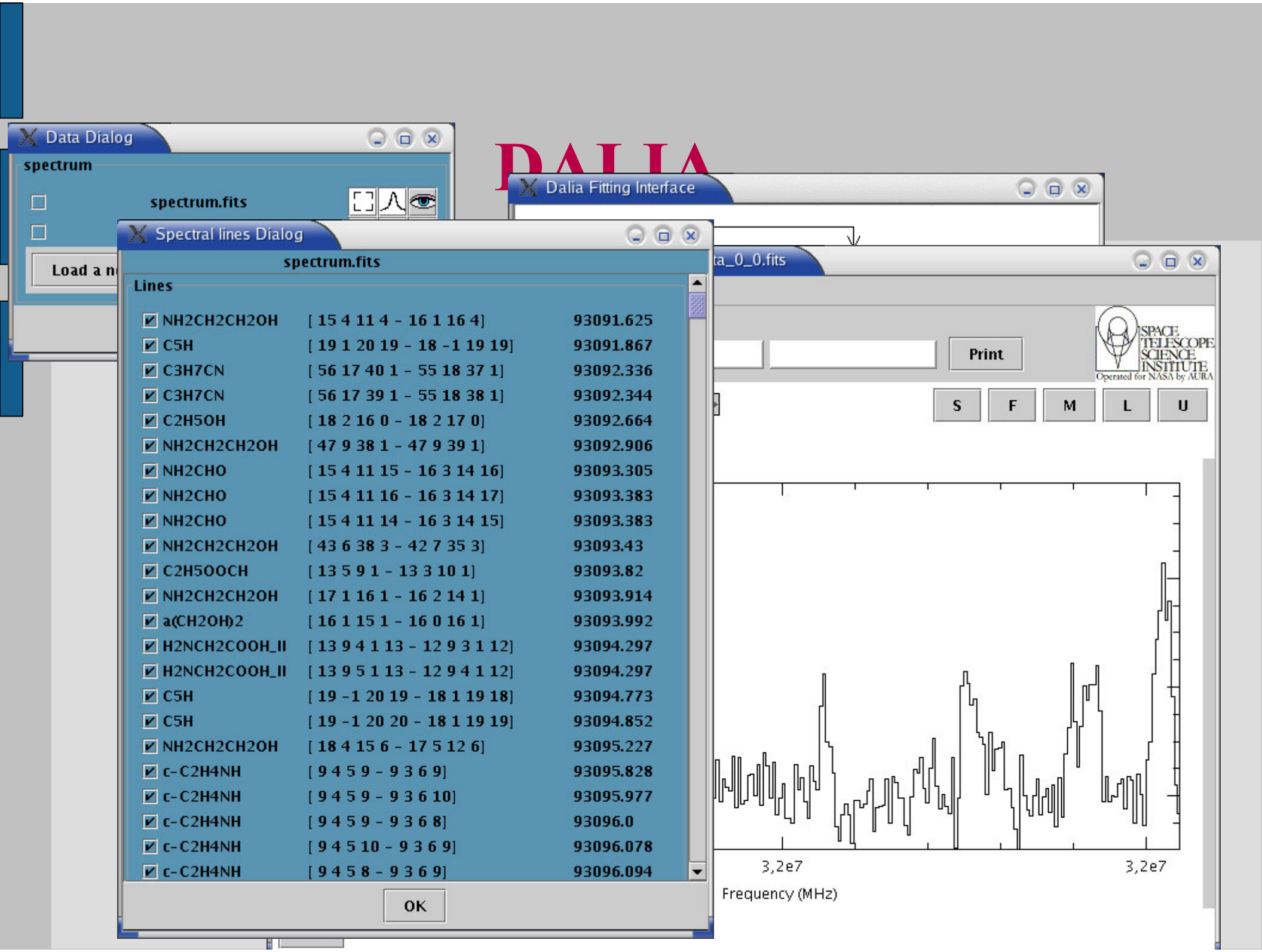
- Query Parameters
  - TARGET, COLLIDER
  - initial_level_energy, final_level_energy
- Return VOTable with
  - List of collisions with TARGET + COLLIDER
  - Link to energy tables (basecol)
  - Link to CDMS values
    - Einstein coefficients, frequency, statistical weight...

Generic Interface to Numerical Codes for Science Data Analysis and Modelling

Frédéric Boone (LERMA)
Marie-Lise Dubernet (LERMA)
Peter Schilke (MPIfR)
Dirk Muders (MPIfR)

Concept


Observations
Use existing formats and visualization tools
Graphical User Interface
model codes
Define a standard
Optimization engine
Use existing algorithms
spectroscopic data
Query existing databases
Best fit parameters with error bars


Data Dialog
spectrum
spectrum.fits
Load a n
Spectral lines Dialog
spectrum.fits
Lines
NH2CH2CH2OH [15 4 11 4 - 16 1 16 4] 93091.625
C5H [19 1 20 19 - 18 -1 19 19] 93091.867
C3H7CN [56 17 40 1 - 55 18 37 1] 93092.336
C3H7CN [56 17 39 1 - 55 18 38 1] 93092.344
C2H5OH [18 2 16 0 - 18 2 17 0] 93092.664
NH2CH2CH2OH [47 9 38 1 - 47 9 39 1] 93092.906
NH2CHO [15 4 11 15 - 16 3 14 16] 93093.305
NH2CHO [15 4 11 16 - 16 3 14 17] 93093.383
NH2CHO [15 4 11 14 - 16 3 14 15] 93093.383
NH2CH2CH2OH [43 6 38 3 - 42 7 35 3] 93093.43
C2H5OOCH [13 5 9 1 - 13 3 10 1] 93093.82
NH2CH2CH2OH [17 1 16 1 - 16 2 14 1] 93093.914
a(CH2OH)2 [16 1 15 1 - 16 0 16 1] 93093.992
H2NCH2COOH_II [13 9 4 1 13 - 12 9 3 1 12] 93094.297
H2NCH2COOH_II [13 9 5 1 13 - 12 9 4 1 12] 93094.297
C5H [19 -1 20 19 - 18 1 19 18] 93094.773
C5H [19 -1 20 20 - 18 1 19 19] 93094.852
NH2CH2CH2OH [18 4 15 6 - 17 5 12 6] 93095.227
c-C2H4NH [9 4 5 9 - 9 3 6 9] 93095.828
c-C2H4NH [9 4 5 9 - 9 3 6 10] 93095.977
c-C2H4NH [9 4 5 9 - 9 3 6 8] 93096.0
c-C2H4NH [9 4 5 10 - 9 3 6 9] 93096.078
c-C2H4NH [9 4 5 8 - 9 3 6 9] 93096.094
OK
Dalia Fitting Interface
ta_0_0.fits
Print
SPACE TELESCOPE SCIENCE INSTITUTE
Operated for NASA by AURA
S
F
M
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3,2e7
3,2e7
Frequency (MHz)

Service for ASAP
(very close to SLAP)

- Query Parameters
  - Frequency_min
  - Frequency_max
  - *Chemical_element*
  - *Chemical_element_symmetry*
- *Return list of transitions with:*
  - *Chemical_element, Chemical_element_symmetry*
  - *Initial_level_energy, Einstein_Coefficient, g_up*
  - *Quantum_number_tag,id_chemical_element,*
  - *Data_source, creation_date*
  - *Link to quantum numbers (URL)*
  - *Link to all collisions with TARGET, to documentation*

Perspective for Atomic and Molecular Data

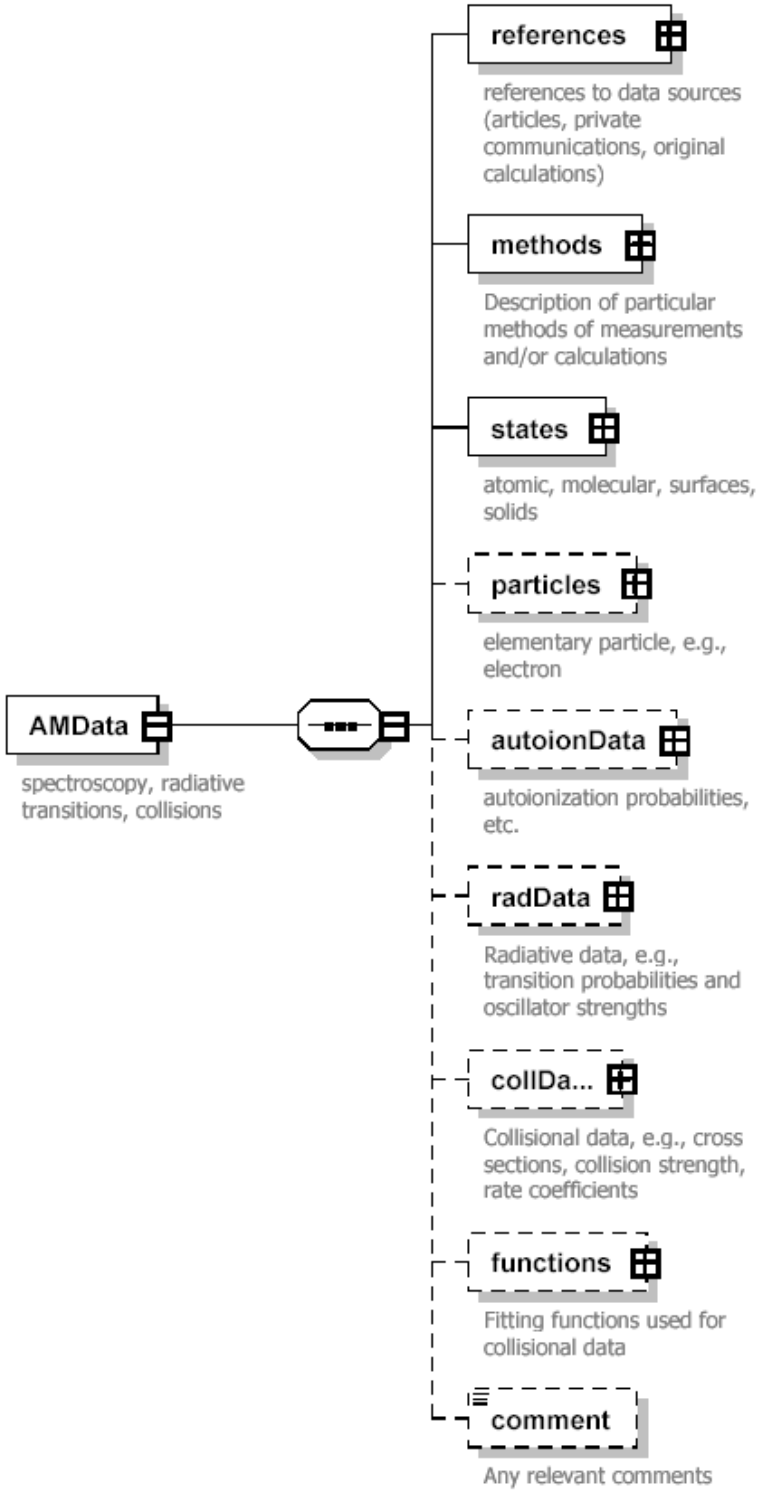
- Access to linelists: well defined – can be implemented

Standardization of Access to other data (ex: rate coefficients of Basecol)

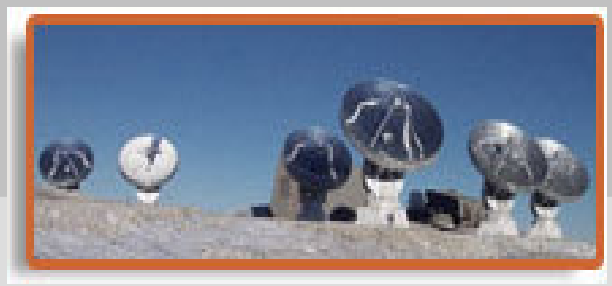
- Working Group of Atomic and Molecular Physicists from NIST, IAEA, Oackridge, NIFS, Paris Observatory (Paper at ICAMDATA, Meudon, Octobre 2006)
- Model will be proposed to IVOA by WG
- Applications: fusion, atmosphere, astrophysics

Building Infrastructure: Atomic and Molecular Data Network--> FP6 or FP7

Paper at ICAMDATA, Meudon, Octobre 2006



Plateau de Bure (IRAM) 6x15m λ=[1, 3] mm

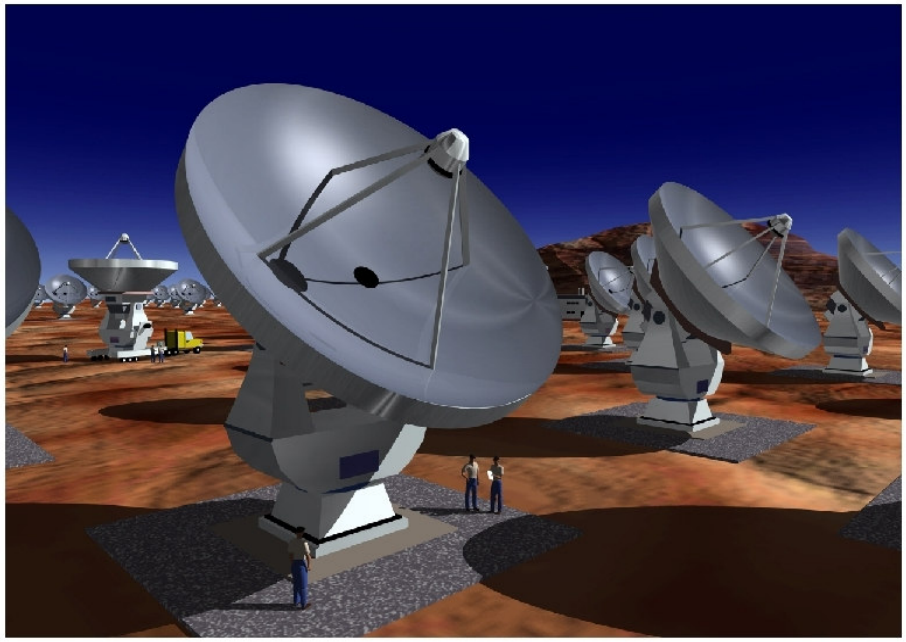


Pico Veleta (IRAM) 30m

SubMillimeter Array (Harvard+Taïwan) 8x6m λ=[0.3, 1.7]mm

Atacama Pathfinder Experiment (MPIfR+ESO) 12m λ=[0.3, 1] mm

Atacama Large Millimeter Array 64x12m λ=[10, 0.35]mm



Herschel (ESA) 3.5m λ=[60, 670]mu

Motivation

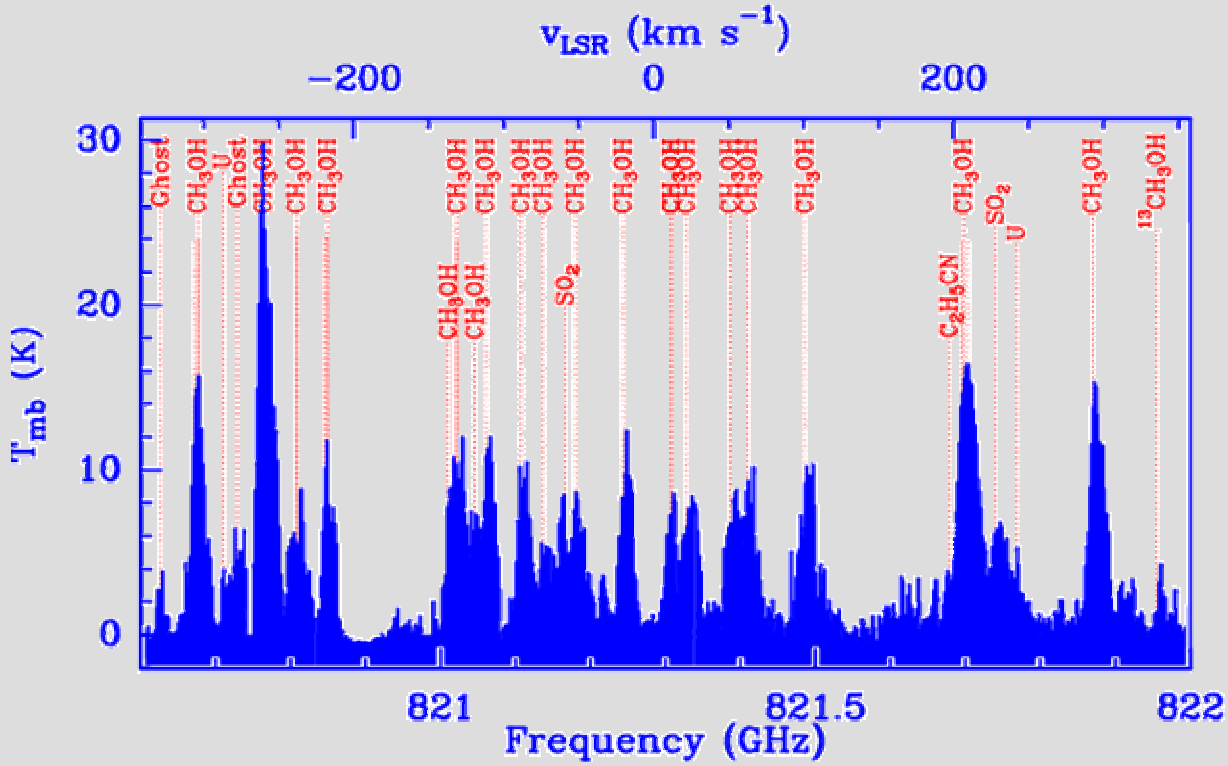
- **New instruments: SMA, APEX, ALMA, Herschel**
  - Great spatial and spectral dynamics
  - Modeling required to extract information
- **Models not available**
  - Not always public
  - Not easily accessible
  - Few of them in data reduction softwares

Motivation

- **Models difficult to use**
  - Need to learn a format or a language
  - Some models are complementary but implemented in different environments, e. g. : dynamics+chemistry+radiative transfer
- **Common needs**
  - Optimization loop to fit the model to the data with **constraints** and error estimation
  - **Interactivity** (control the model parameters)
  - Spectroscopic data --> query spectro databases

Example I – Line surveys

- **Early stage of star formation: Hot Core**
  - Extremely rich chemistry triggered by high temperature and density and enriched by the evaporation of the icy mantles of grains
    -> “line forest”
  - Submm range privileged:
    - High energy transitions
    - Light hybrids (OH, CH, H2O...) have fundametal level in submm
    - Infrared pumping -> measure of background

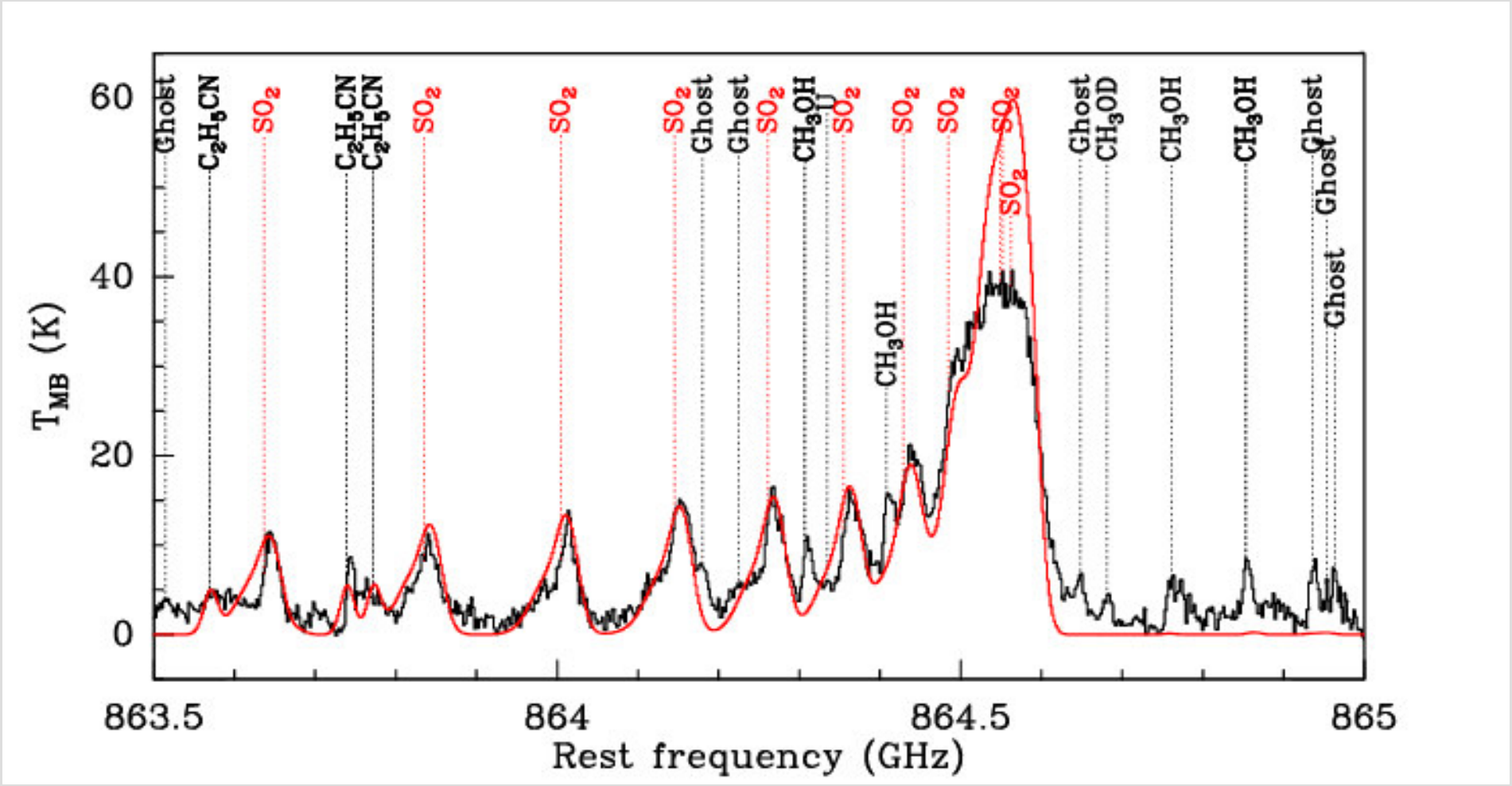

v_{LSR} (km s^{-1})
−200
0
200
30
20
10
0
T_{mb} (K)
Ghost
CH_3OH
U
Ghost
CH_3OH
CH_3OH
CH_3OH
CH_3OH
CH_3OH
CH_3OH
CH_3OH
CH_3OH
CH_3OH
CH_3OH
SO_2
CH_3OH
CH_3OH
CH_3OH
CH_3OH
CH_3OH
CH_3OH
CH_3OH
CH_3OH
C_2H_5CN
CH_3OH
SO_2
U
CH_3OH
$^{13}CH_3OH$
821
821.5
822
Frequency (GHz)

ANALYSIS OF THE DATA

- ✔ *the whole spectrum is fitted at once (Schilke et al. 1997)*
- ✔ *LTE using molecular database (JPL, Cologne)*
- ✔ *fits source size, T_{ex}, column density, line width and velocity*
- ✔ *fits all lines of a species and isotopomers at once*
  ⇒ ***takes intra-species line blends and optical depth effects explicitly into account!***
- ✔ *fits all species at once* ⇒ ***takes inter-species line blends into account!***

Claudia Comito 2003, PhDT

GOOD FIT: SO_2



Claudia Comito 2003, PhDT

Example II – protostellar collapse

Collapse model

↓

Radial profiles

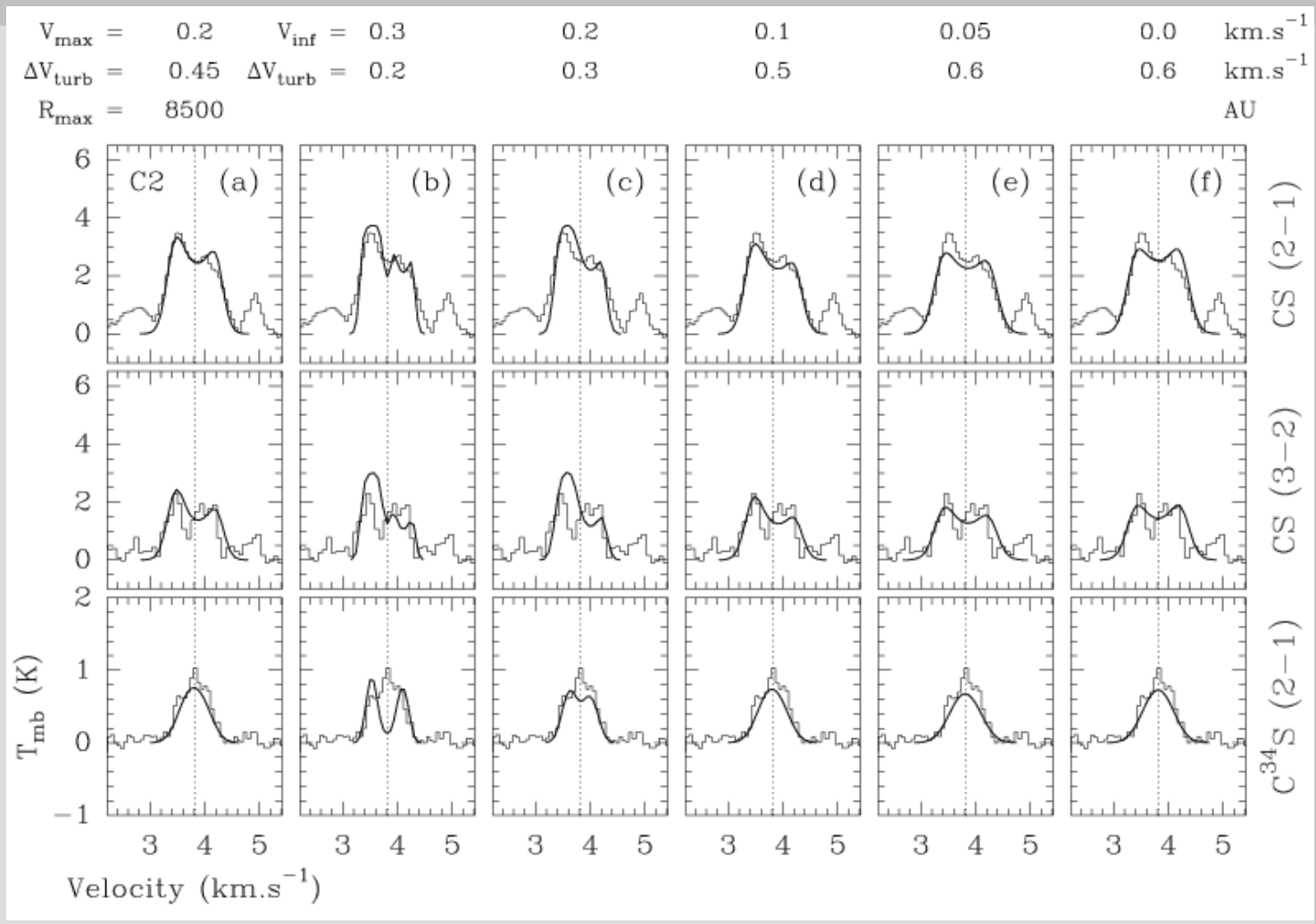
Temperature
Density
velocity

↓

Radiative Transfer
BERNES-MAPYSO

↓

Simulated spectra



Arnaud Belloche 2002, PhDT

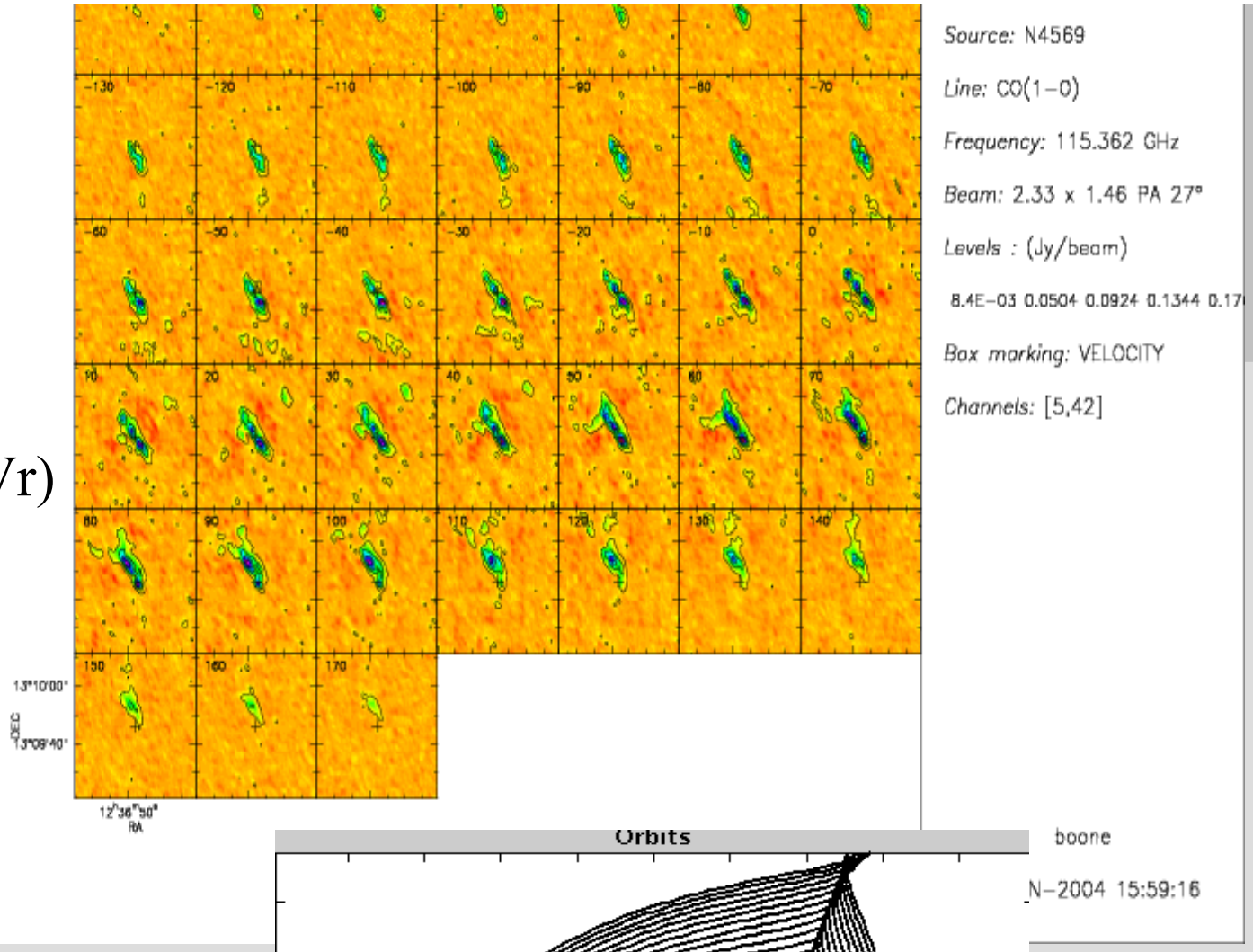
Example III – Galactic dynamics

- **Gas kinematics in the center of galaxies**
  - Evolution of galaxies
  - AGN fueling
  - Black Hole growth
  - Starburst/AGN connection

Example III – Galactic dynamics

- **NUGA survey** (PI: S. Garcia-Burillo, F. Combes)
  - Survey of 12 nearby active galaxies with IRAM Plateau de Bure Interferometer CO(1-0) and CO(2-1)
  - Get a new insight into the dynamics of the inner 1kpc
    with a resolution <100pc
- **Kinematic modeling**
  - Use assumptions on orbits to reproduce observations
  - The aim is to “deproject” the data to obtain a 6D description

3D
(RA, Dec, Vr)



6D
(X, Y, Z, Vx, Vy, Vz))

Examples summary

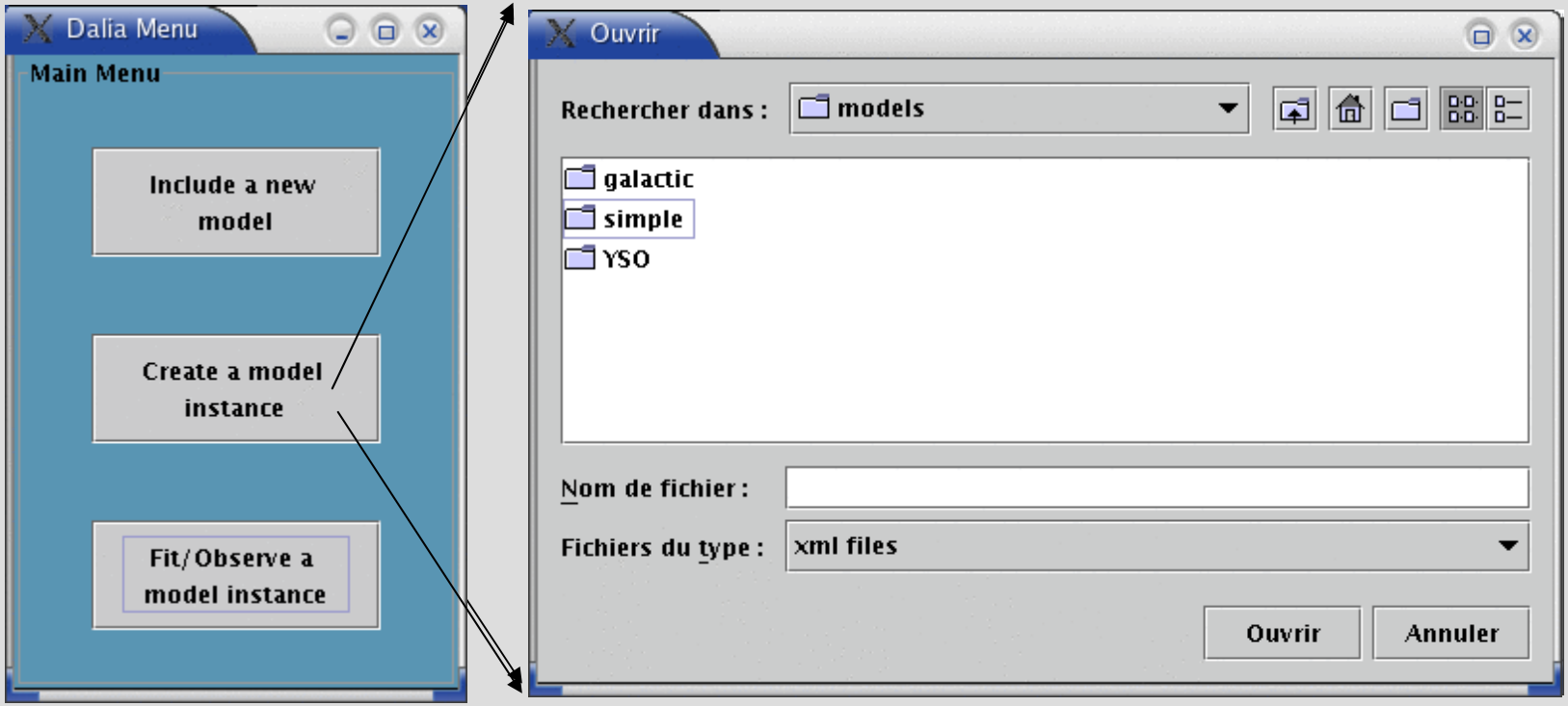
- **EX I (line surveys)**
  - Link to spectroscopic databases
  - Ability to easily control a large number of params
  - Radiative transfer
- **EX II (protostellar envelops)**
  - Several models in line (dynamics + radiative transf.)
  - Several kinds of data (spectra+images)
- **EX III (galactic dynamics)**
  - Need ability to compare different kinematic models to data cubes

A prototype, DALIA
(Direct Approach to Spectral LIne Analysis)

- **Main functionalities**
  - Edit parameters of a model to create a first guess
  - Fit the model to the data (1D, 2D, 3D ....) via optimization
  - Constrain the parameters
  - Include spectroscopic data from molecular databases
  - Allow to introduce any new model code (Fortran, C...)
- **Implementation**
  - GUI in JAVA
  - Description of models in XML following a “schema”
  - Interface GUI/models: ASCII for params and FITS for data
  - Visualization: Specview (spectra) Jimage (2d & 3d)

DALIA

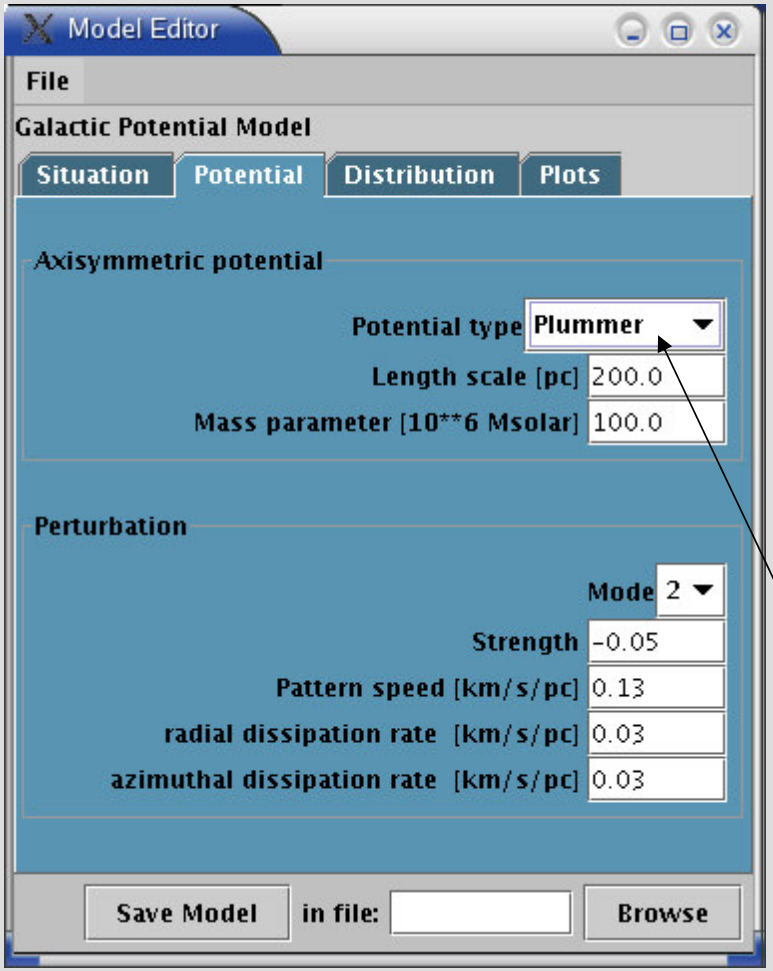
- Create a model instance (first guess)

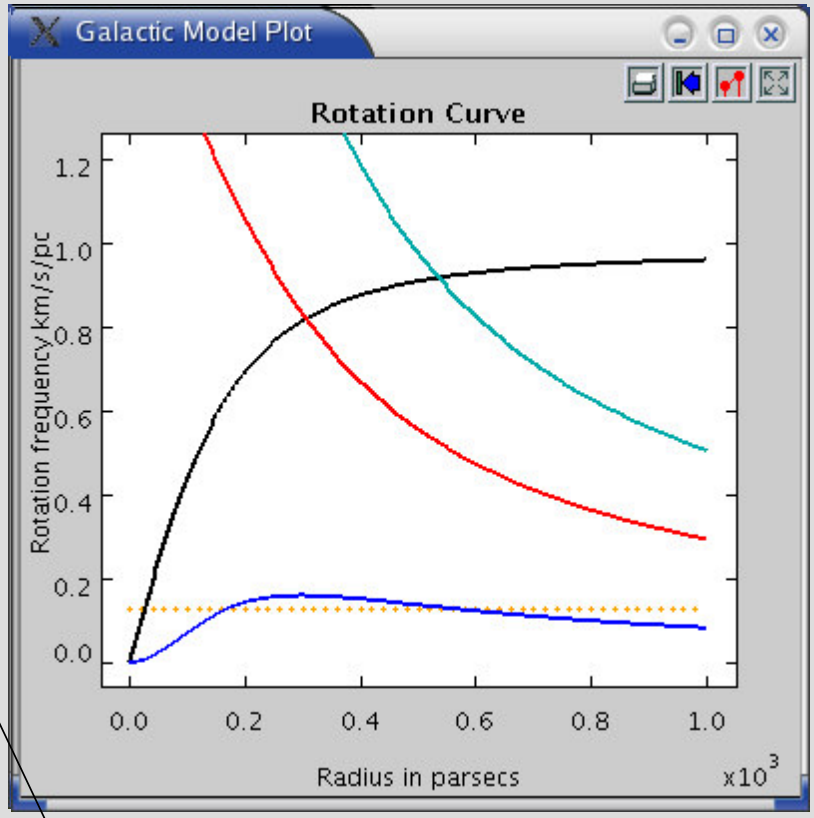


DALIA

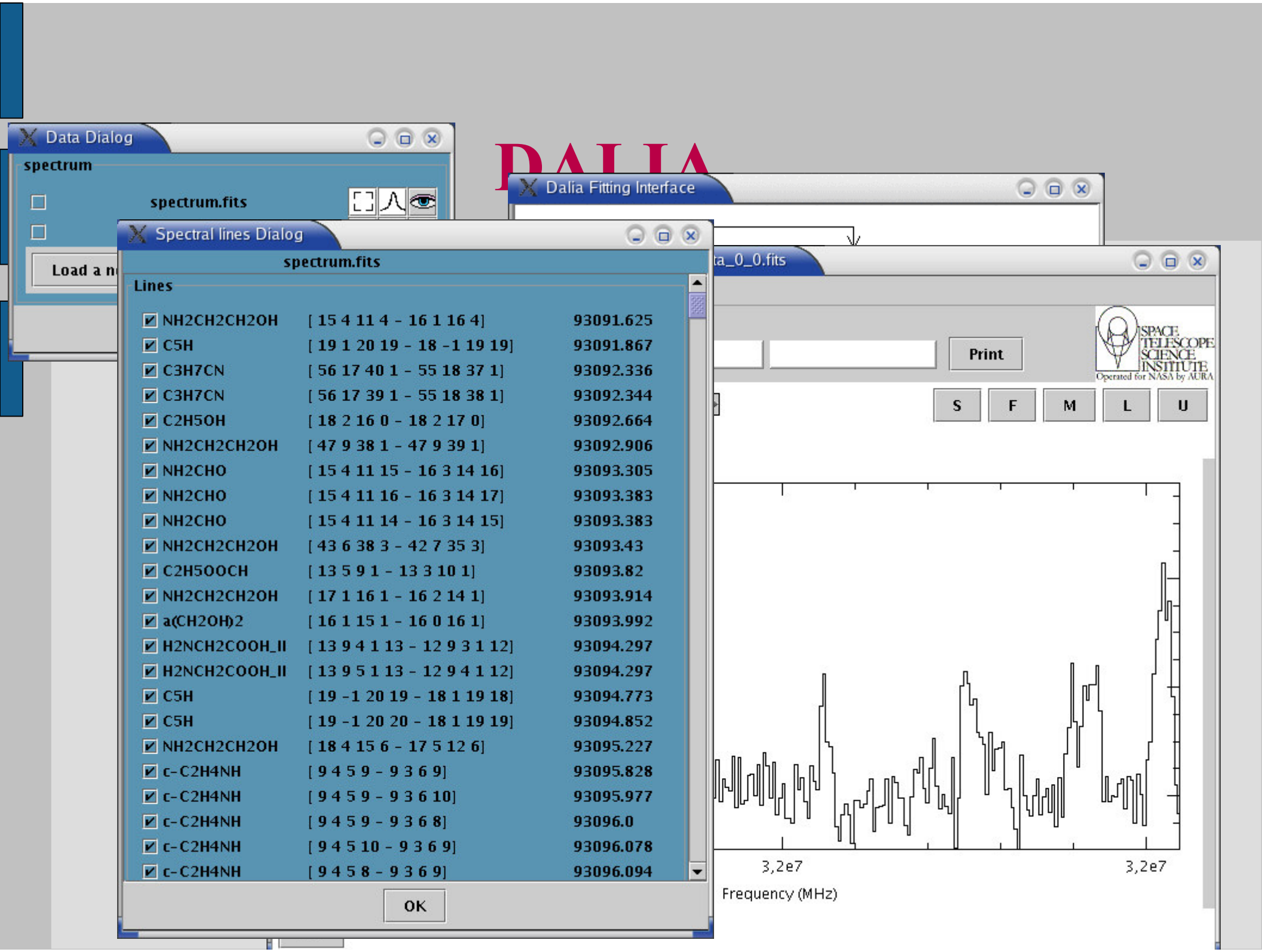
- Create a model instance of a galactic model

GUI generated by the XML description of the model





Choices


Data Dialog
spectrum
spectrum.fits
Load a n
Spectral lines Dialog
spectrum.fits
Lines
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C5H [19 1 20 19 - 18 -1 19 19] 93091.867
C3H7CN [56 17 40 1 - 55 18 37 1] 93092.336
C3H7CN [56 17 39 1 - 55 18 38 1] 93092.344
C2H5OH [18 2 16 0 - 18 2 17 0] 93092.664
NH2CH2CH2OH [47 9 38 1 - 47 9 39 1] 93092.906
NH2CHO [15 4 11 15 - 16 3 14 16] 93093.305
NH2CHO [15 4 11 16 - 16 3 14 17] 93093.383
NH2CHO [15 4 11 14 - 16 3 14 15] 93093.383
NH2CH2CH2OH [43 6 38 3 - 42 7 35 3] 93093.43
C2H5OOCH [13 5 9 1 - 13 3 10 1] 93093.82
NH2CH2CH2OH [17 1 16 1 - 16 2 14 1] 93093.914
a(CH2OH)2 [16 1 15 1 - 16 0 16 1] 93093.992
H2NCH2COOH_II [13 9 4 1 13 - 12 9 3 1 12] 93094.297
H2NCH2COOH_II [13 9 5 1 13 - 12 9 4 1 12] 93094.297
C5H [19 -1 20 19 - 18 1 19 18] 93094.773
C5H [19 -1 20 20 - 18 1 19 19] 93094.852
NH2CH2CH2OH [18 4 15 6 - 17 5 12 6] 93095.227
c-C2H4NH [9 4 5 9 - 9 3 6 9] 93095.828
c-C2H4NH [9 4 5 9 - 9 3 6 10] 93095.977
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OK
Dalia Fitting Interface
ta_0_0.fits
Print
SPACE TELESCOPE SCIENCE INSTITUTE
Operated for NASA by AURA
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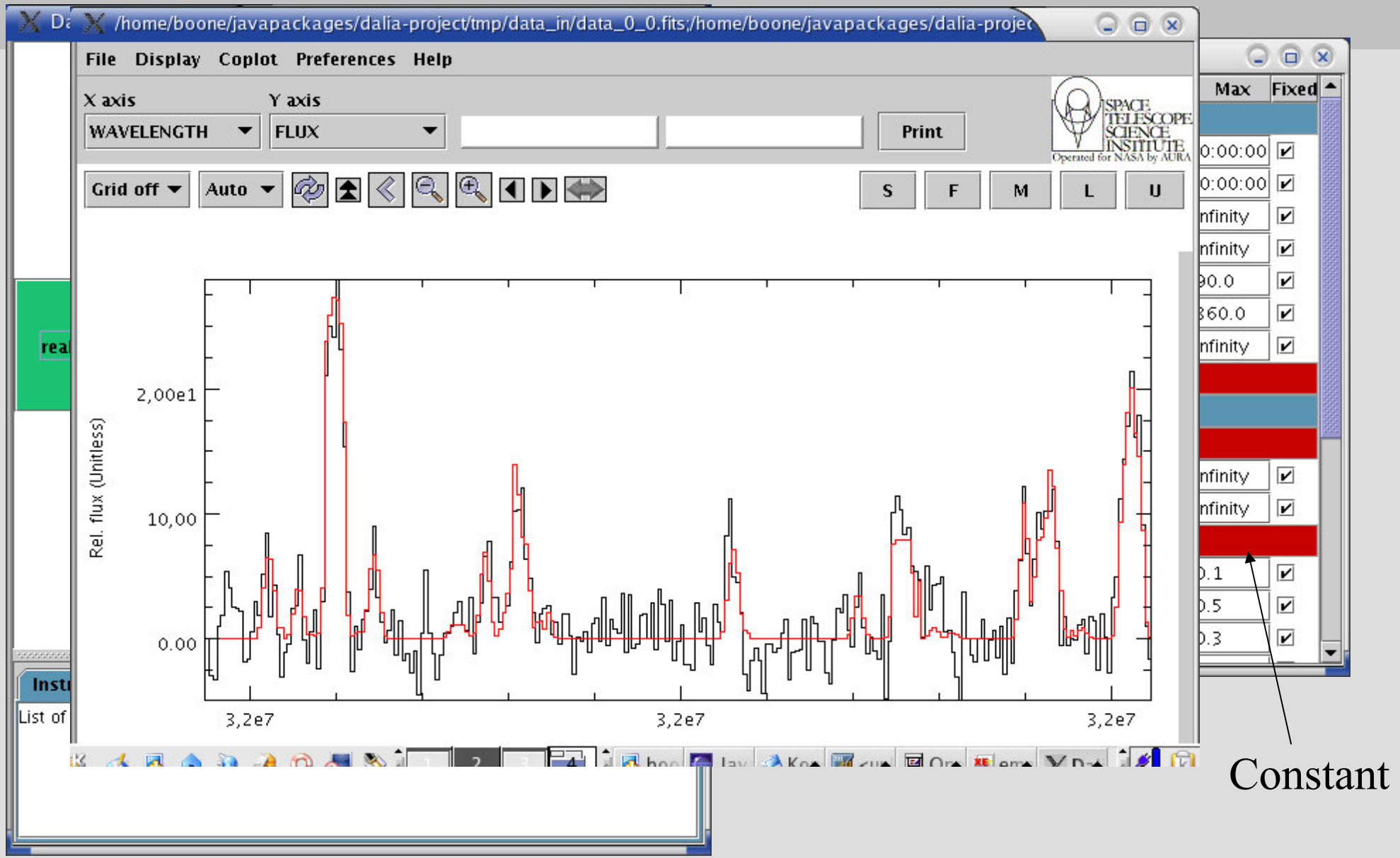
F
M
L
U
3,2e7
3,2e7
Frequency (MHz)

DALIA


/home/boone/javapackages/dalia-project/tmp/data_in/data_0_0.fits;/home/boone/javapackages/dalia-projec
File
Display
Coplot
Preferences
Help
X axis
WAVELENGTH
Y axis
FLUX
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SPACE TELESCOPE SCIENCE INSTITUTE
Operated for NASA by AURA
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Rel. flux (Unitless)
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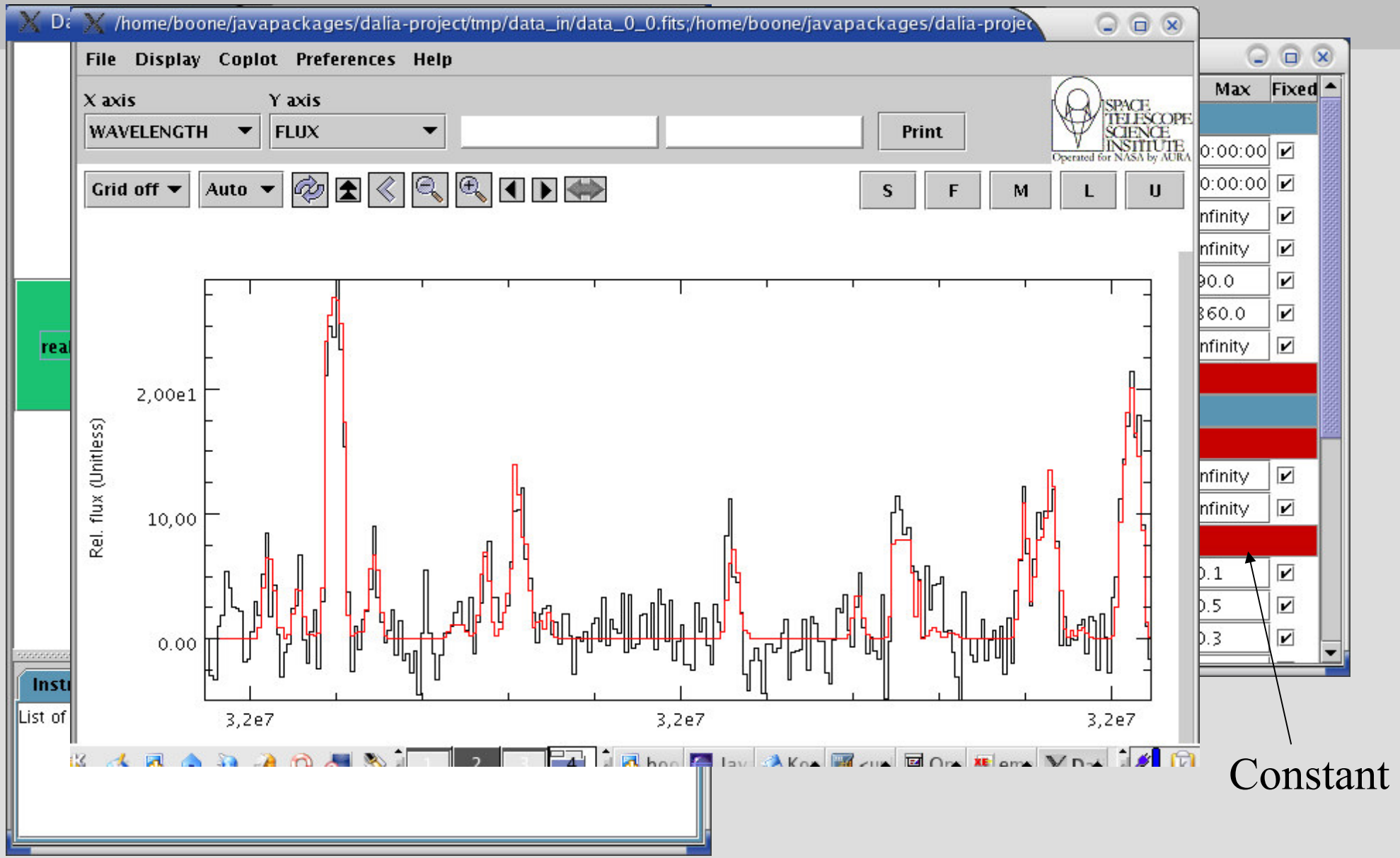
10,00
0.00
3,2e7
3,2e7
3,2e7
Max
Fixed
Constant

DALIA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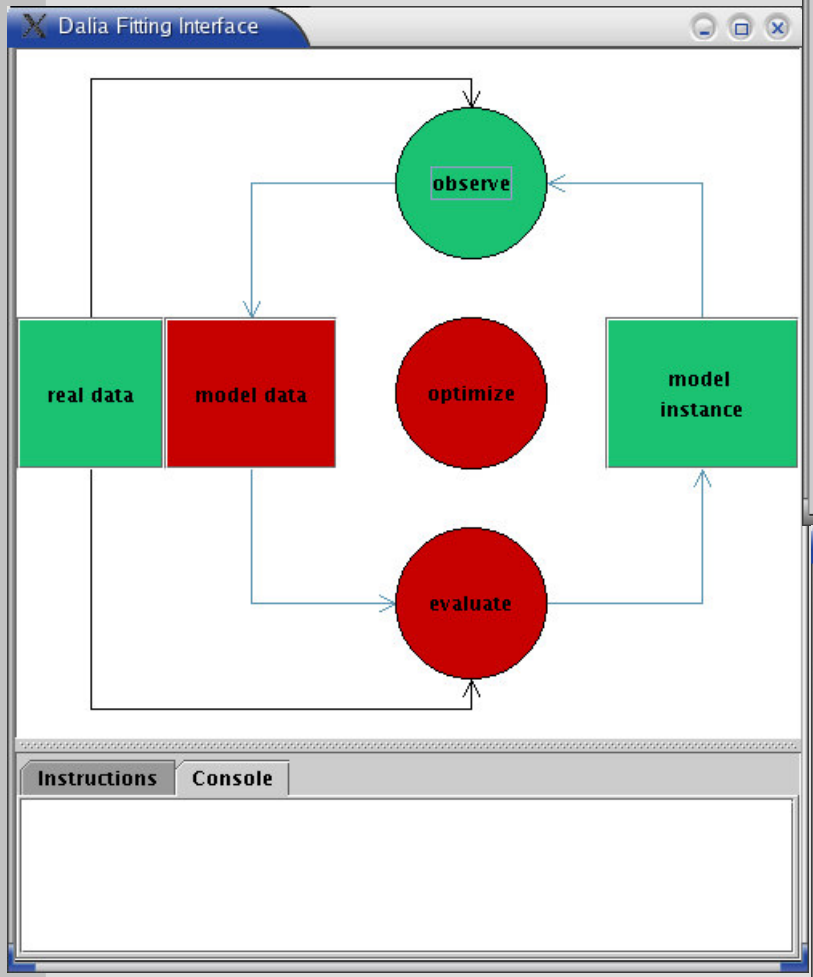
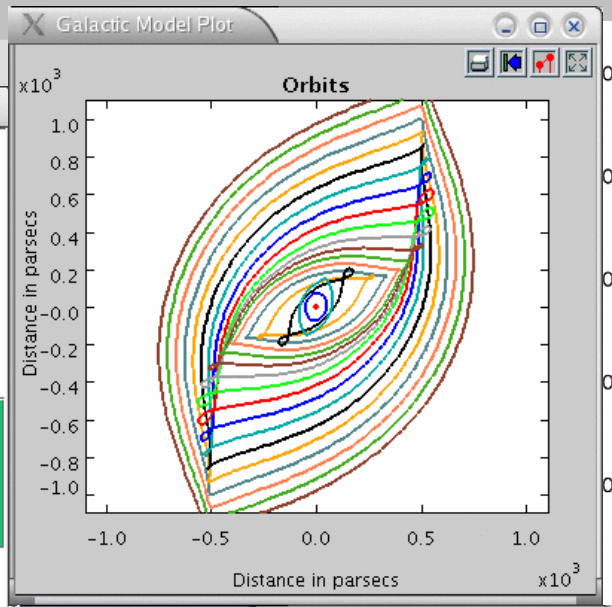
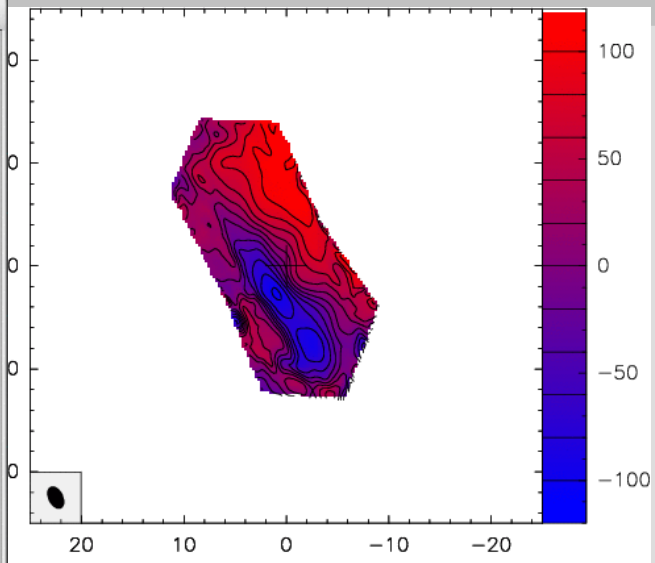
3,2e7
Max
Fixed
Constant

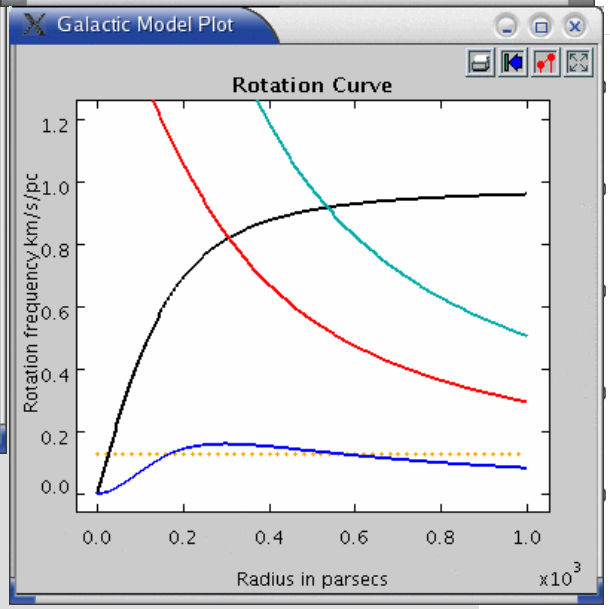
DALIA

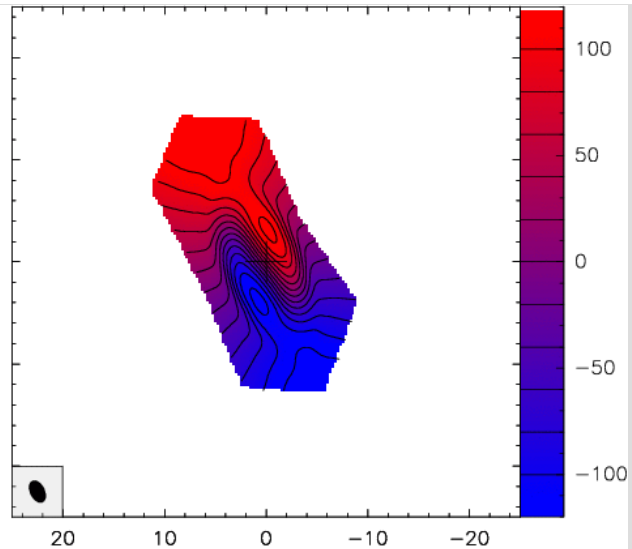
NGC 4569







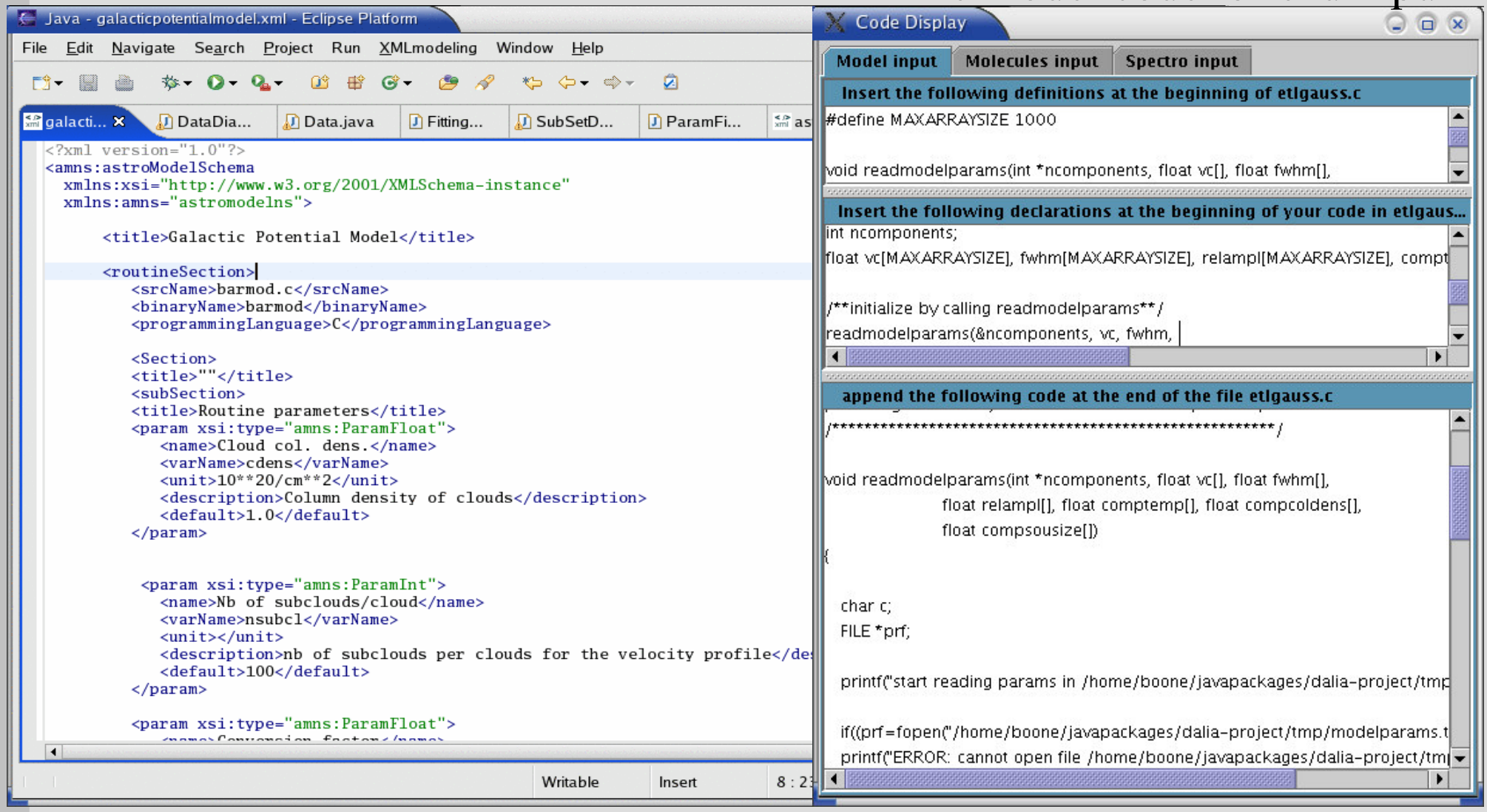




DALIA

XML file describing the model

Pieces of C-code be included in the model code to read input



Summary

- **new generation of software for science analysis and knowledge sharing**
- **a concept: “wrapping rather than re-inventing”**
- **DALIA, JAVA interface with most of the functionalities soon complete**
- **Remains to include**
  - use different models in line, e.g. Dynamics+Radiative Transfer
    --> **interoperability, workflow**

Outlook

- **Generic software**
  - Any data (1D, 2D, 3D,...), any model
  - Standard for models --> Virtual Observatory
  - Can also be used for simulation (Monte Carlo)
  - All wavelengths and not only astronomy
- **Possible extensions**
  - Association with computing resources: server (web service), parallel computing
  - Association with archive facilities (VO) for the data but also for the model codes and the model instances

Outlook

- **ASAP could become a very general VO software to interface codes**
- **Models should be well documented**
- **Development open to the community**
  MPIfR + Observatoire de Paris +Strasbourg+...