Data, Databases, Tools for Alma and Virtual Observatories

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(Data: Rate coefficients, Basecol, MAGIX/ASAP, VO)
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CESR, Toulouse, FR

Supported by CNRS, EU (Molecular Universe FP6- RTN), French Virtual Observatory

European Research Training Network-FP6 molecular universe

molecular-universe.obspm.fr

Data (FP6 program on Thursday)

see 2006 Summerschool

- Spectroscopic data:
  - Carbon chains, PAH
- Reactions (lab. & theory)
  - Carbon chains, PAH
- Rate coefficients for excitation processes

(cf talk at IAU "Astrochemistry" , 2005, Asilomar)

- DBB/Tools: CDMS, UMIST, BASECOL, CASSIS

Rate coefficients for excitation processes

Collisions with He, H_2

CH^+, H_2O, HDO, NH_3, SO($^3\Sigma$), SiO, SO_2, N_2H^+, H_2CO, HC_3N

CO, CN ($^2\Sigma$), CS, SiS

CH3OH

Next :

Carbon chains, organic molecules

High Temperature and bending modes

High Accuracy = Heavy CPU

See Poster 28: Wernli & al (HC_3N)

Requirements for Tools Implementation (I)

VO: Interoperability of ressources in order to produce science (http://www.ivoa.net)

- Observational Data
  - Archives: well taken care in IVOA, cross correlation (ALMA working group)
- Theoretical/Observed Microphysics Data in Databases
  - Ex : CDMS/JPL, BASECOL, LOVAS catalogues, UMIST, etc ....
- Numerical Codes
  - Ex : Radiative transfert codes, Modelling codes
- Analysis tools/Visualisation
  - Analysis software (reduction pipeline, optimization algorithms, synthetic spectra): CASSIS, ASAP/MAGIX, etc ....

Requirements for Tools Implementation (II)

VO: Interoperability of ressources in order to produce science (www.ivoa.net)

- Full description of all data
  - Microphysics:
    - references, methods, accuracy
    - Identify measurements/calculations from extrapolation
  - Codes:
    - Identify hypothesis, algorithms, parameters
- Use standardized exchange langage
- Long term maintenance
- Deal with various sources: **Basecol database** (rates with H, He, H_2), Leiden database (rates with H_2) --> F. Schoïer, CDMS --> H. Müller, JPL, etc...

Basecol Database
http://www.obspm.fr/basecol

ML Dubernet
LERMA, Paris Observatory

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Past Contributors: B. Debray[**], G. Souemes[*]

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Basecol Database
http://www.obspm.fr/basecol
Useful for astrophysicists and physicists
Published (de)-excitation rate coefficients

- Rotational (fine, hyperfine)
- Ro-vibrational, Vibrational
- Currently: 21 Target molecules
- Perturbers : He, H, H_2 (not exhaustive)
- 76 collisional systems

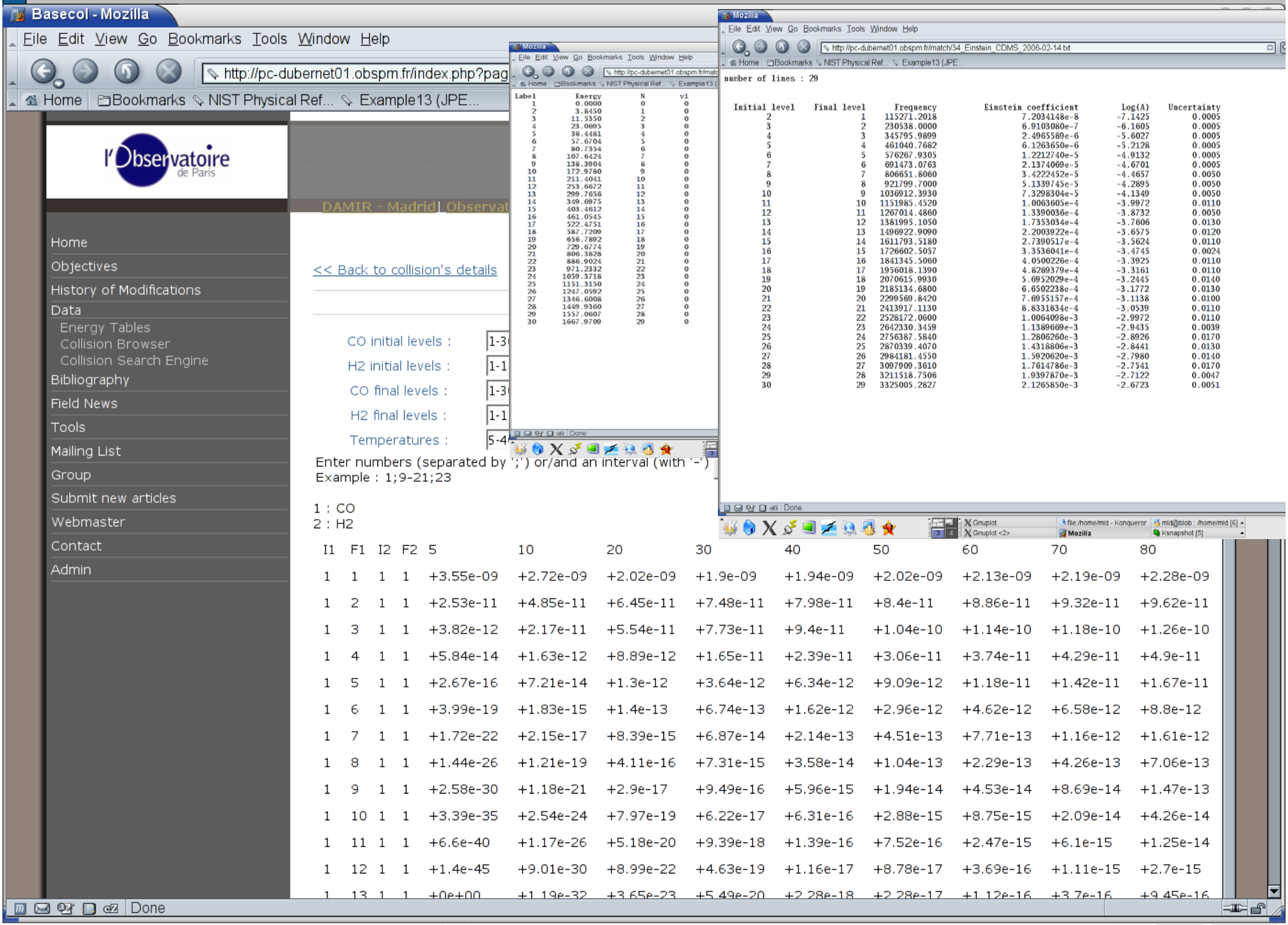
- Fully documented and referenced (630 ref.)

- Linked to
  - CDMS or JPL
  - Theoretical energy levels

- Fitting coefficients, Visualisation tools
- Under Test: NH_3, CH_3CN

Quality Control

- Origin of Data : All papers carefully read
- Tables in Database
  - Careful check by detailed balance, *F. Daniel*
    - Rate coefficients and fitting functions
    - Theoretical energy levels
- Long term maintenance
  - Team of physicists
  - Software engineer and VO-Paris Data Center
- Official opening: Published paper (June 06)



Label	Energy	N	v1
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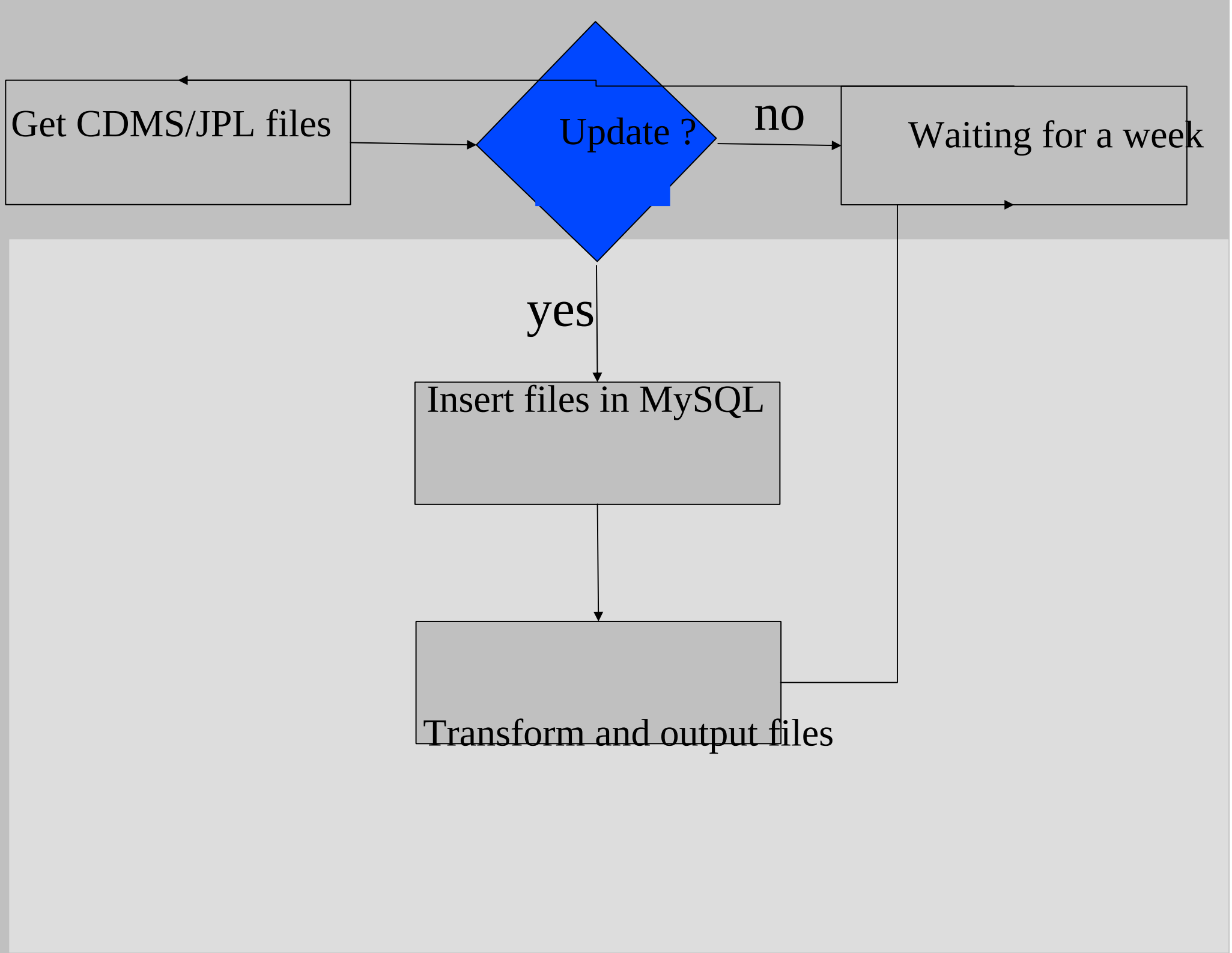
2	3.8450	1	0
3	11.5350	2	0
4	23.0695	3	0
5	38.4481	4	0
6	57.6704	5	0
7	80.7354	6	0
8	107.6424	7	0
9	138.3904	8	0
10	172.9780	9	0
11	211.4041	10	0
12	253.6672	11	0
13	299.7656	12	0
14	349.6975	13	0
15	403.4612	14	0
16	461.0545	15	0
17	522.4751	16	0
18	587.7209	17	0
19	656.7892	18	0
20	729.6774	19	0
21	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

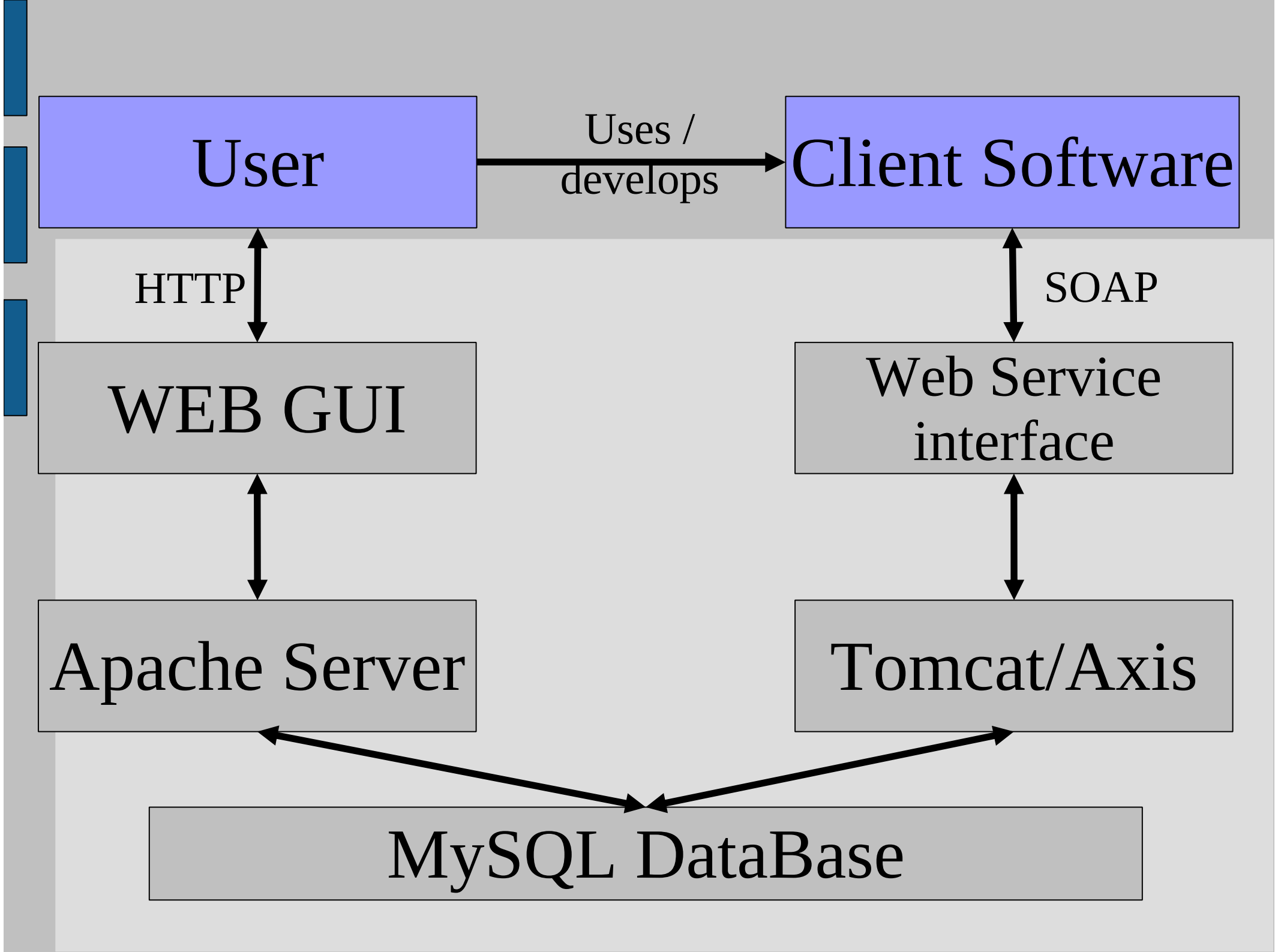
http://pc-dubernet01.obspm.fr/match/34_Einstein_CDMS_2006-02-14.txt

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

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


Get CDMS/JPL files
Update ?
no
Waiting for a week
yes
Insert files in MySQL
Transform and output files


User
Uses / develops
Client Software
HTTP
SOAP
WEB GUI
Web Service interface
Apache Server
Tomcat/Axis
MySQL DataBase

AUTOMATIC ACCESS

Basecol Web Service

- Query for a single molecule
  - Query for a process
  - Query for a collider
  - Query for a temperature range
- Get
  - Rate coefficients
  - Theor. and experim. energy levels
  - Einstein coeff. and statist. weights
  - Errors
  - Fits
  - Documentation

Client for MOLPOP (M. Elitzur)

Get collisions, CDMS/JPL

- Retrieve all data or some data
- Return VOTable and ascii files
- mol.lev, mol.aij, mol_col1.kij, mol_col2.kij
- Create a file with all names

Link to PDR:

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, stat. weight...

EXCHANGE LANGAGE= XML
OUTPUT FORMAT NOT AN ISSUE

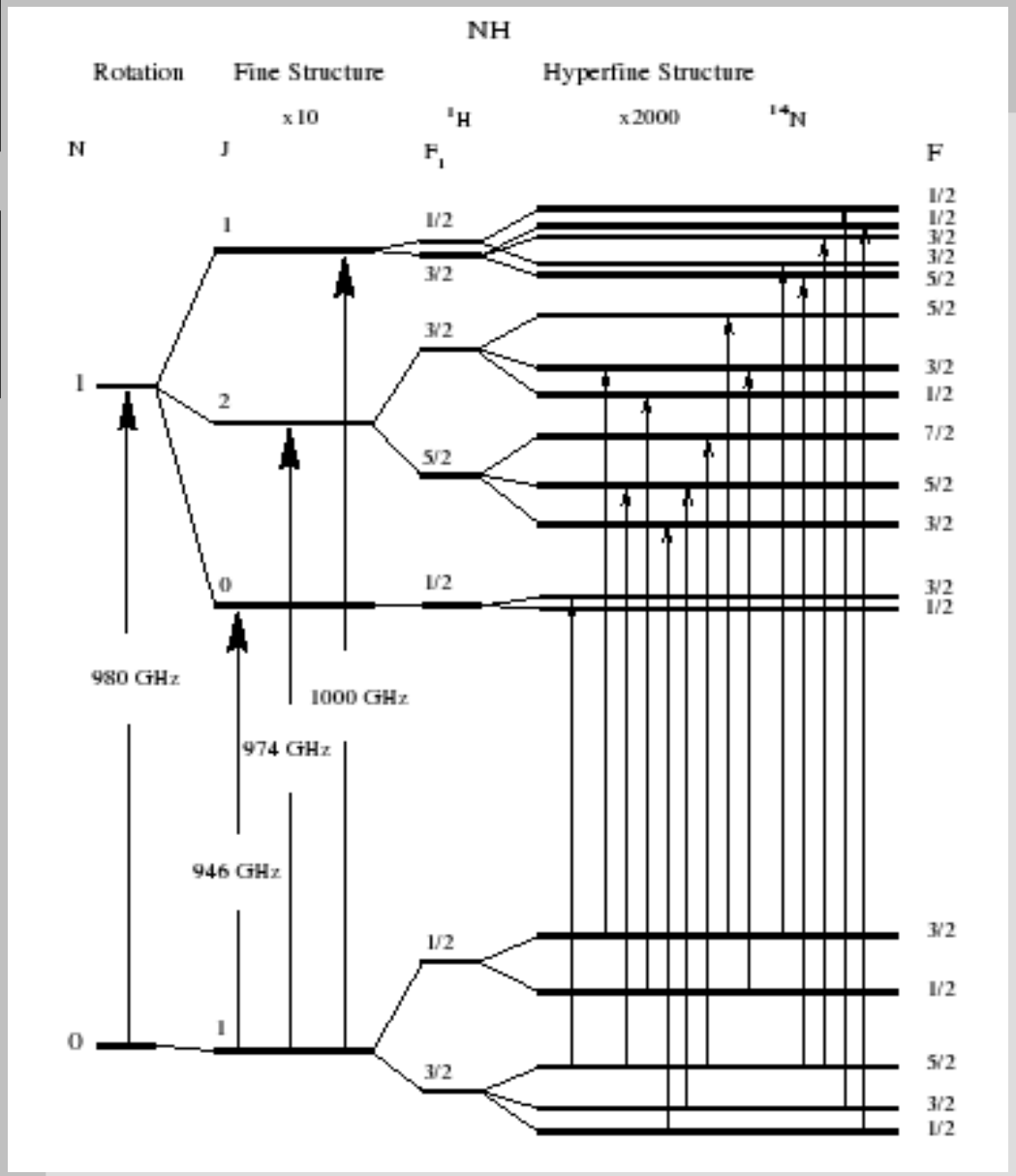
Service for ASAP/MAGIX

(very close to SLAP)

Get all CDMS/JPL + BASECOL

- 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*

Spectral Line Access Protocol
IVOA standard : SLAP

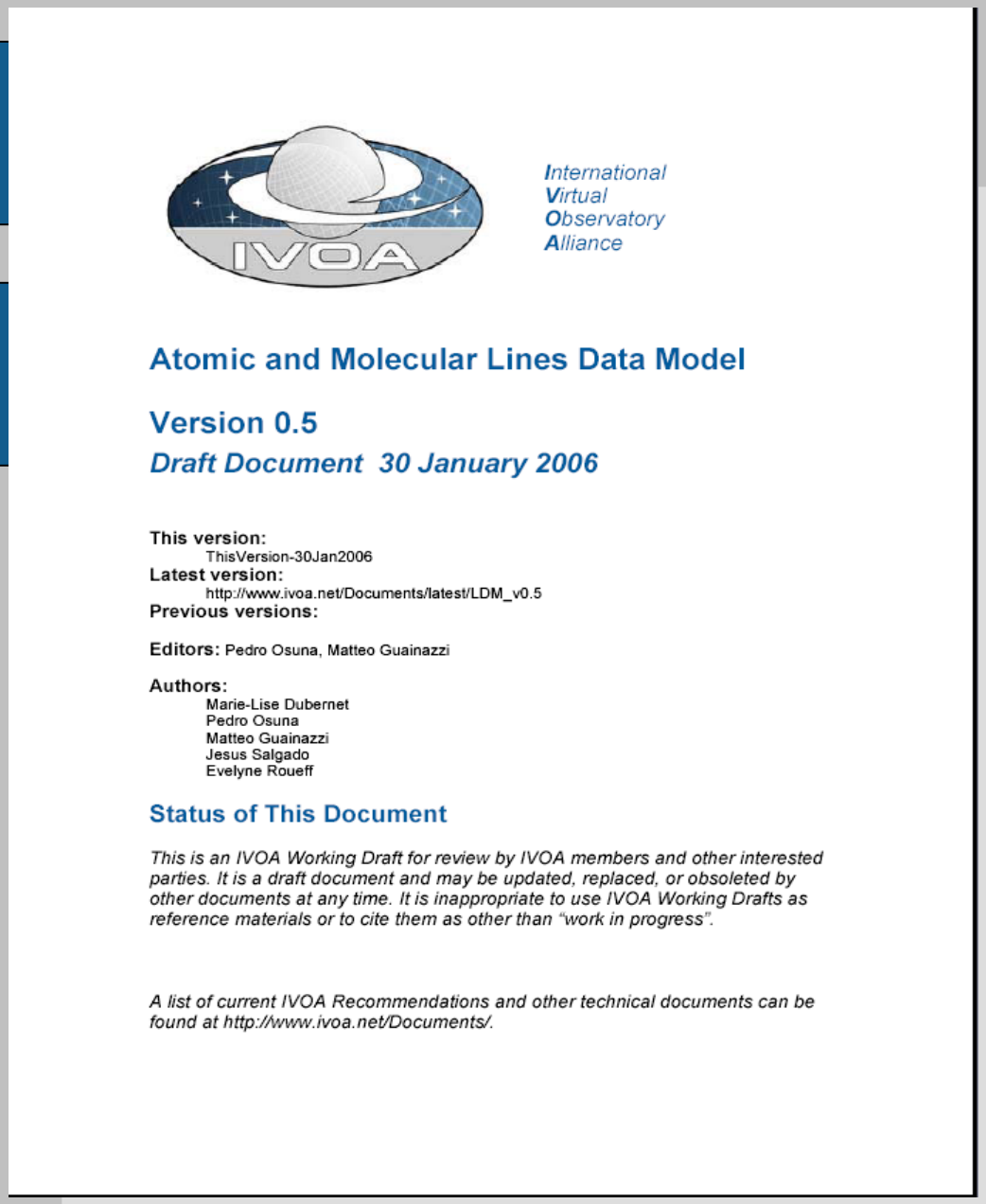


Paris Observatory and ESA/ESAC

ML Dubernet, P. Osuna, M. Guanazzi, J. Salgado, E. Roueff

MLD acknowledges support from VO-France, MDA project (F. Genova), Paris Observatory

Atomic and Molecular Lines Data Model



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:

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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**

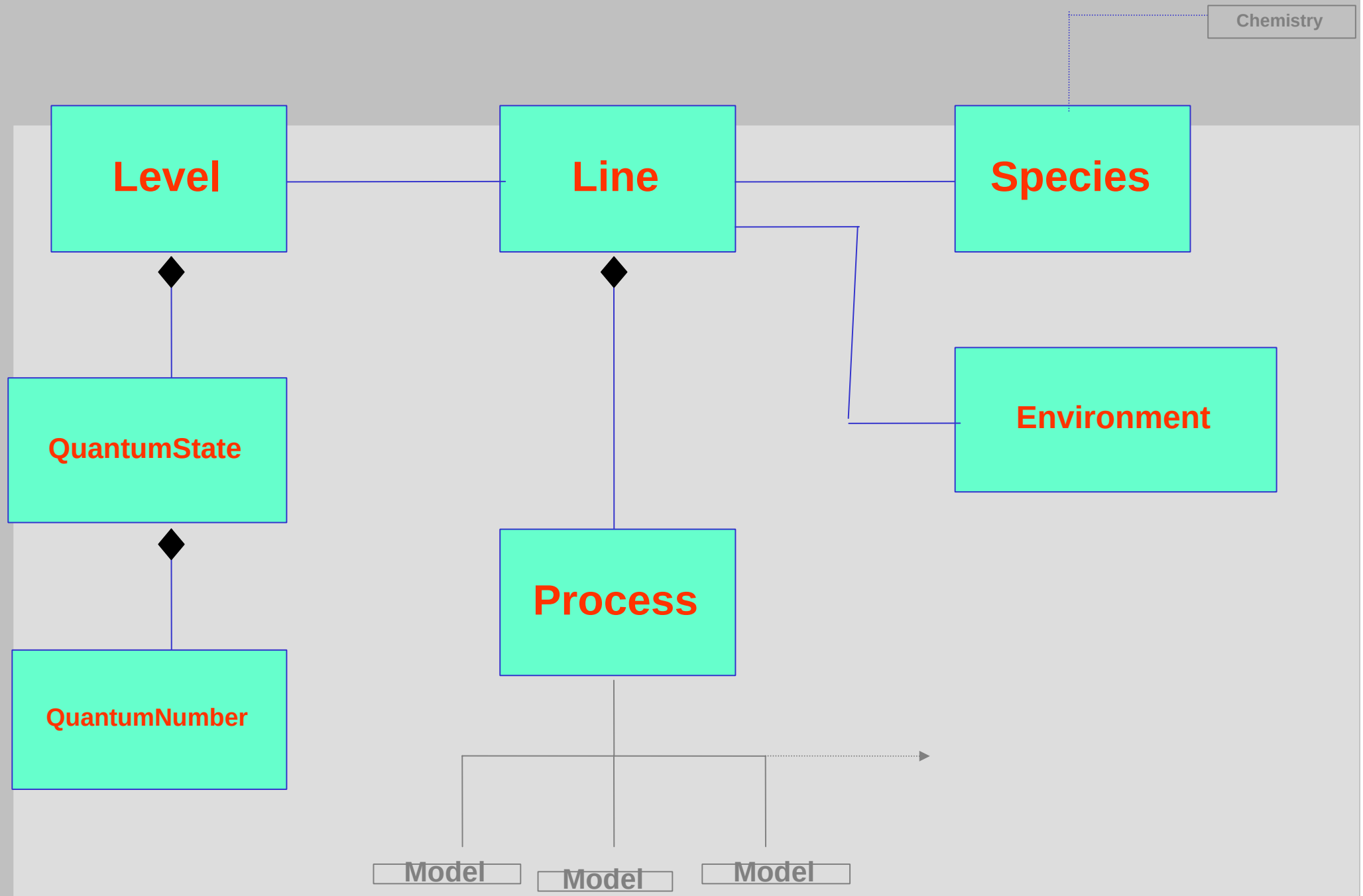
- **circulated to the DM and DAL groups, as well as to atomic and molecular astrophysicists for comments**

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

- **Useful for ETL studies and calibration**

- **Starting document for ALMA working group (Linelists)**

Structure

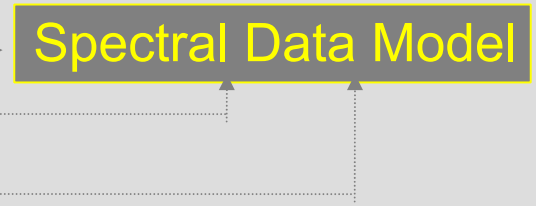

Chemistry
Level
Line
Species
QuantumState
Environment
Process
QuantumNumber
Model
Model
Model

Line

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

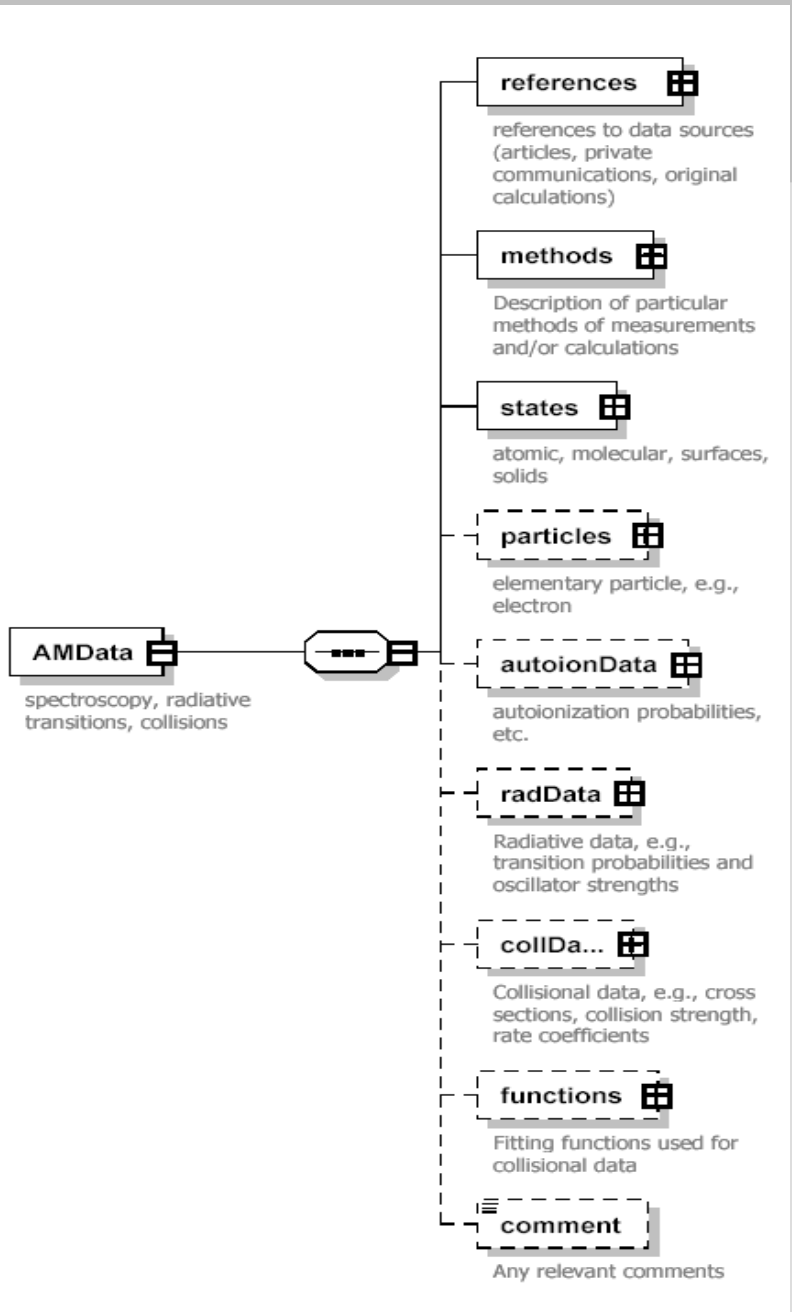
Attributes:

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



Perspective for Atomic and Molecular Data

- Access to linelists: **SLAP is currently implemented on CDMS/JPL (all QN properly identified, symmetry)**
- **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



Generic Interface to Numerical Codes for Science Data Analysis and Modelling

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

Motivation

- New instruments: large amount of data
- Provide an interface
  - with an number of « public codes »
  - With different analysis tools
  - With various visualisation tools
  - For individuals to use with their private codes (public?)
  - For a collaboration to implement complementary codes such as 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)***
- ***Molecular data --> query molecular databases***

Examples summary

- **EX I (line surveys)**
  - Link to spectroscopic/rate coefficients databases
  - Ability to easily control a large number of params
  - Radiative transfer
- **EX II (protostellar envelopes)**
  - 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

Example II – protostellar collapse

Collapse model

↓

Radial profiles

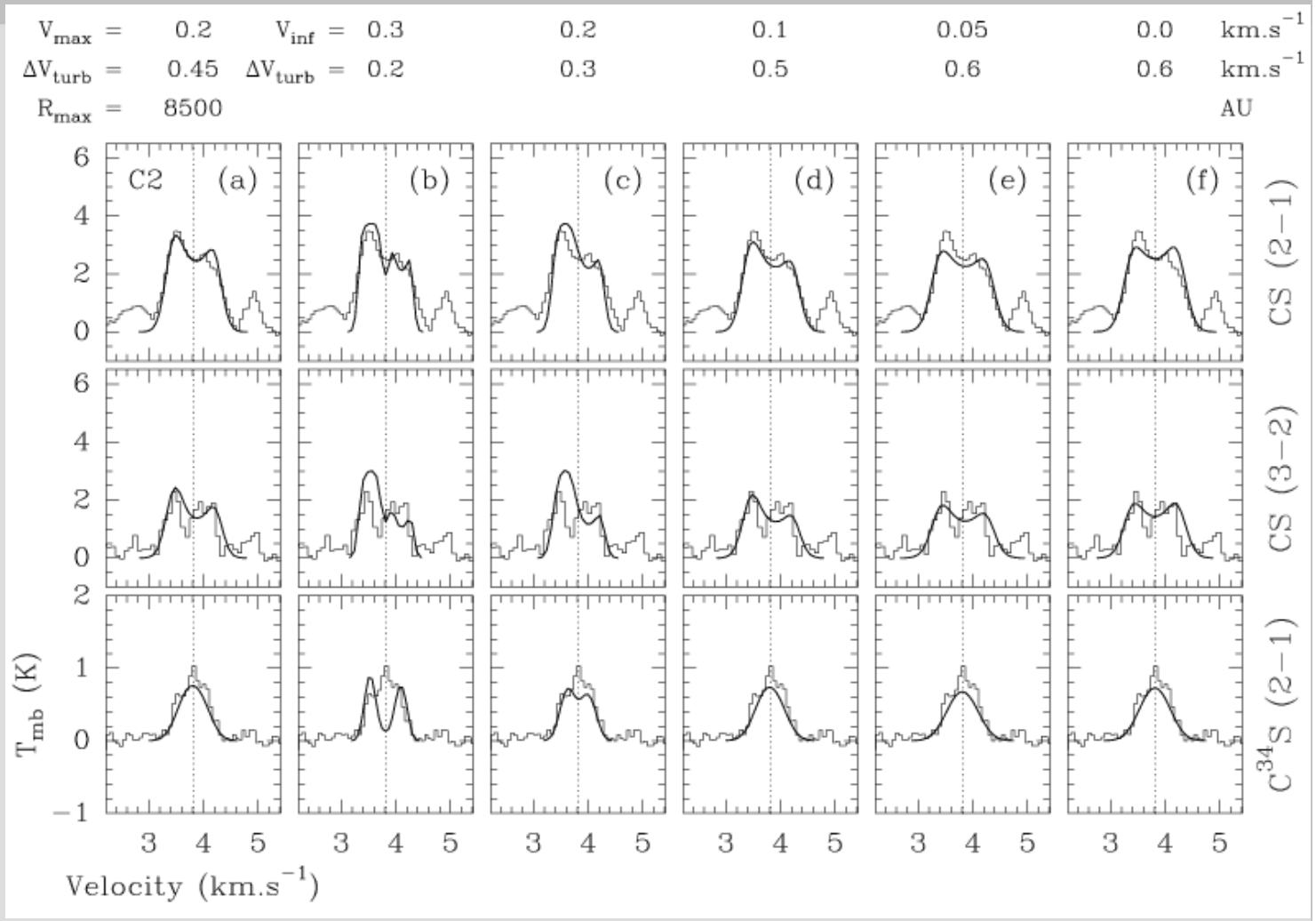
Temperature
Density
velocity

↓

Radiative Transfer
BERNES-MAPYSO

↓

Simulated spectra



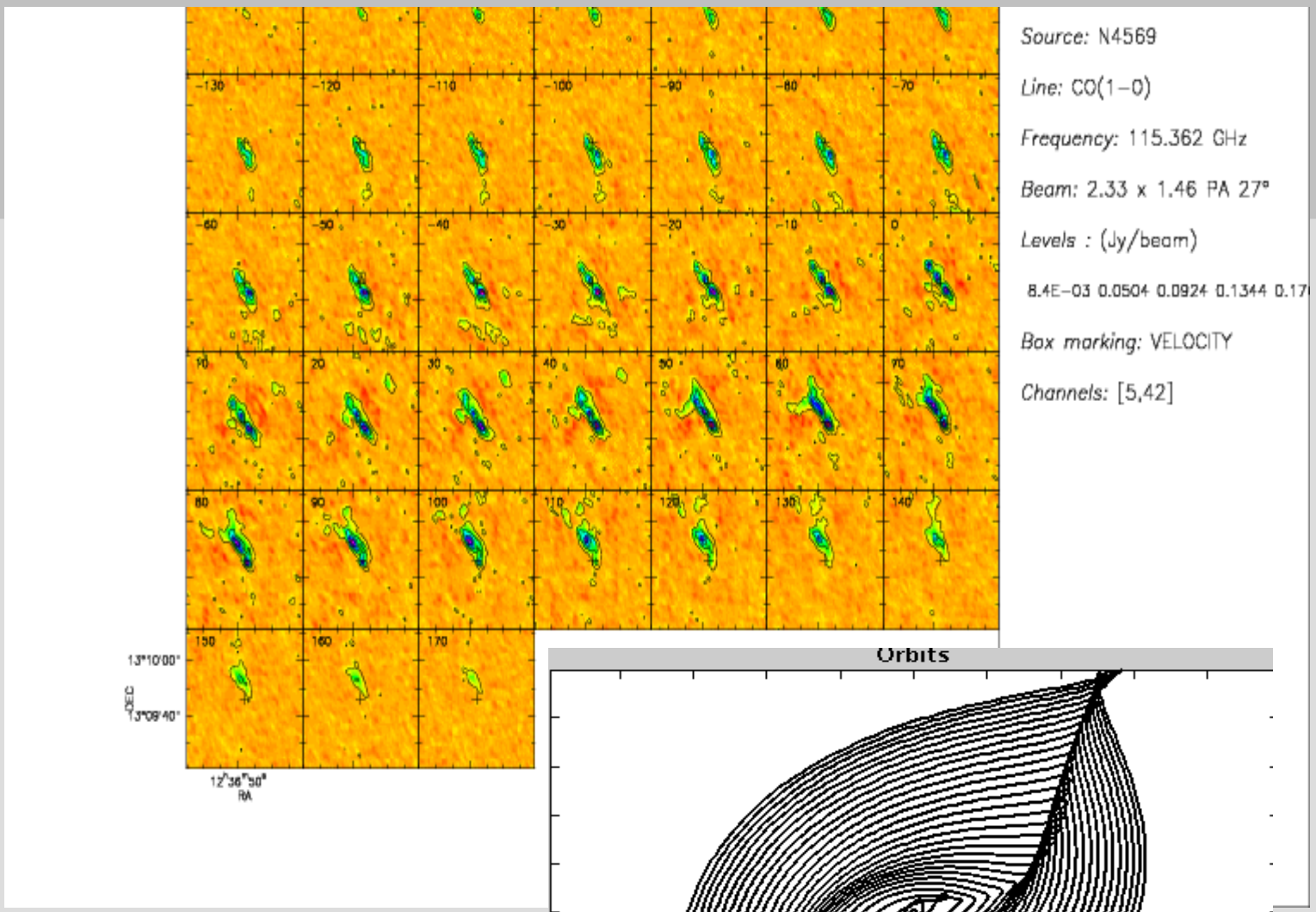
Arnaud Belloche 2002, PhDT

Example III – Galactic dynamics

- **Gas kinematics in the center of galaxies**
  - Evolution of galaxies, AGN fueling, Black Hole growth, Starburst/AGN connection
- **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)
- **Kinematic modeling**
  - Use assumptions on orbits to reproduce observations
  - The aim is to “deproject” the data to obtain a 6D description

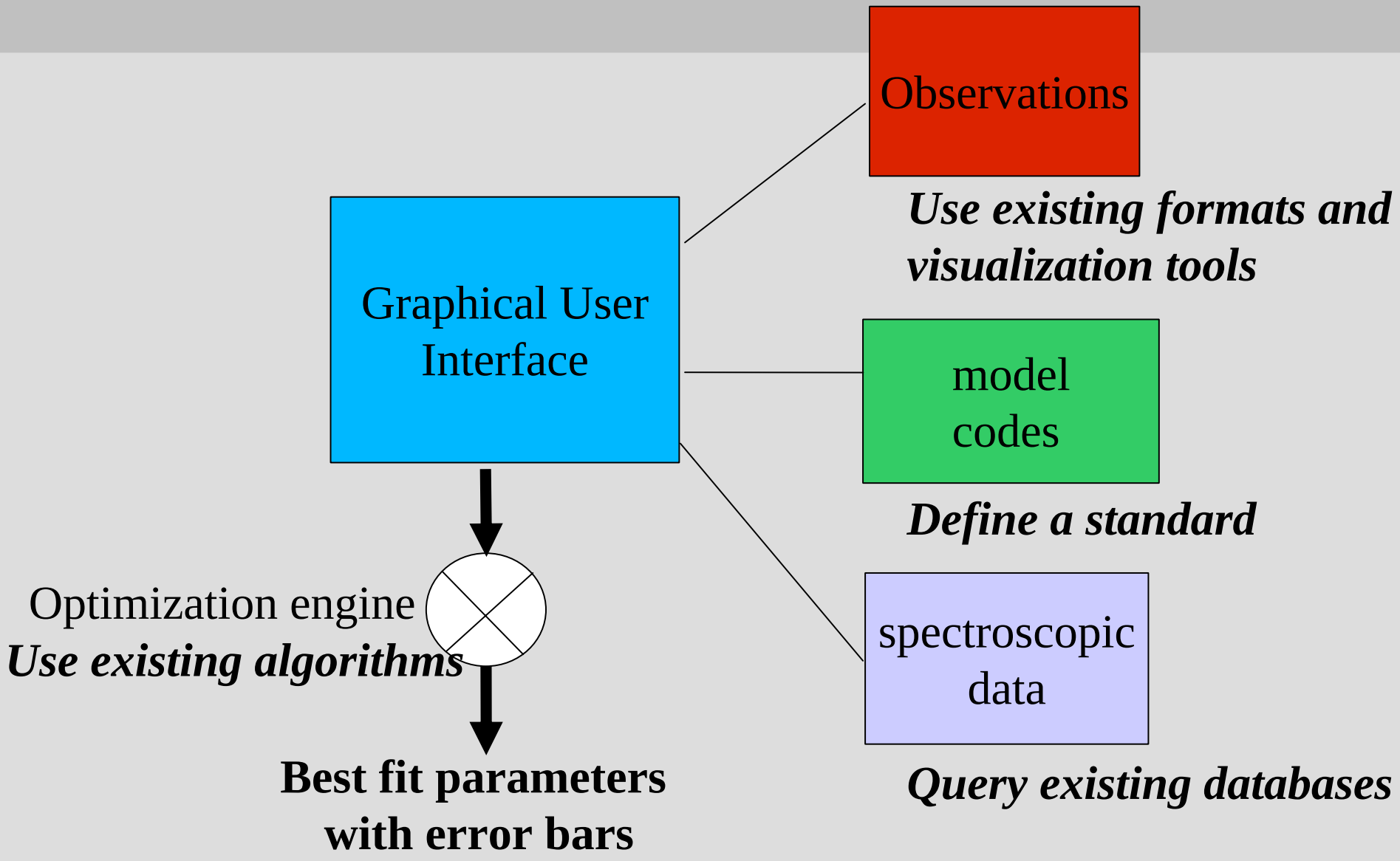
Example III – Galactic dynamics

3D
(RA, Dec, Vr)



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

Concept

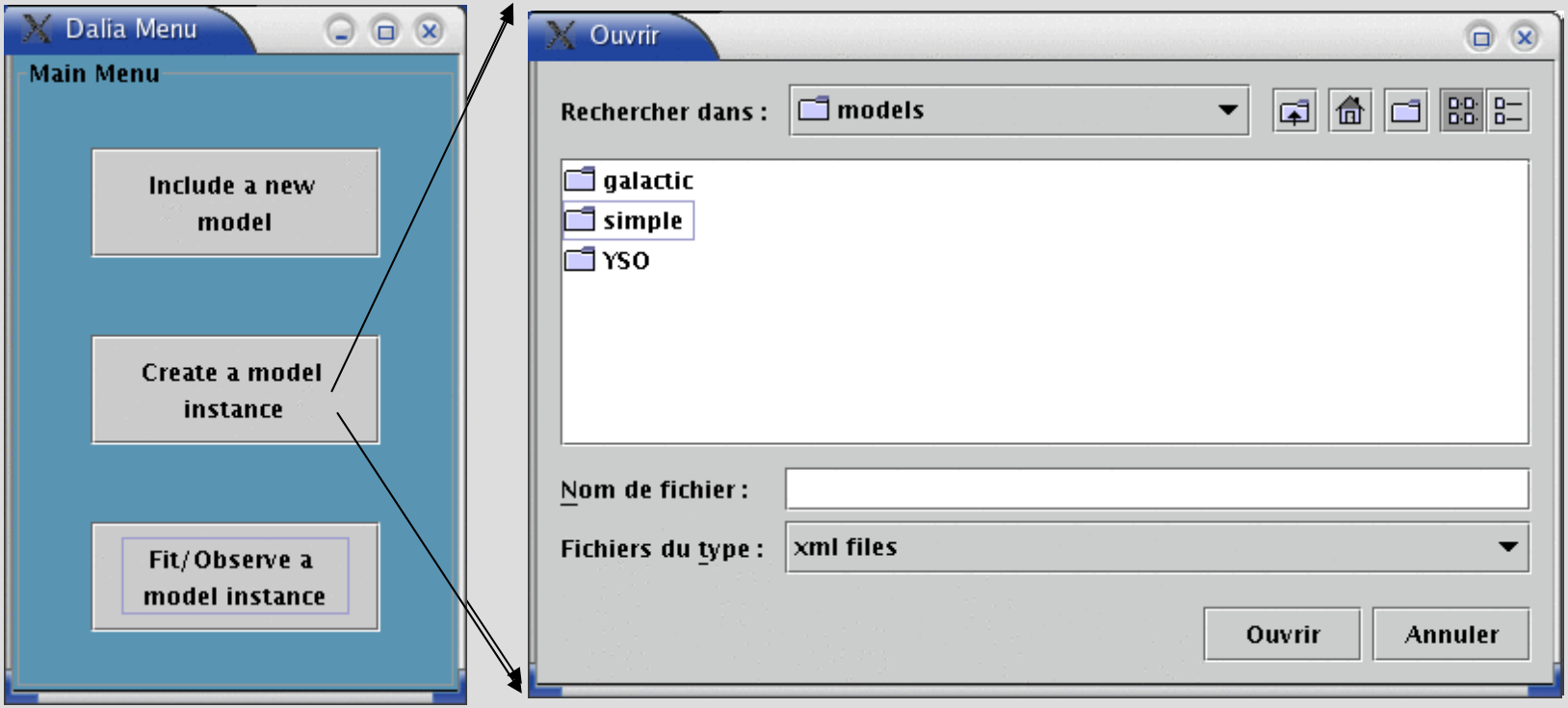

Observations
Use existing formats and visualization tools
Graphical User Interface
model codes
Define a standard
Optimization engine
Use existing algorithms
spectroscopic data
Best fit parameters with error bars
Query existing databases

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

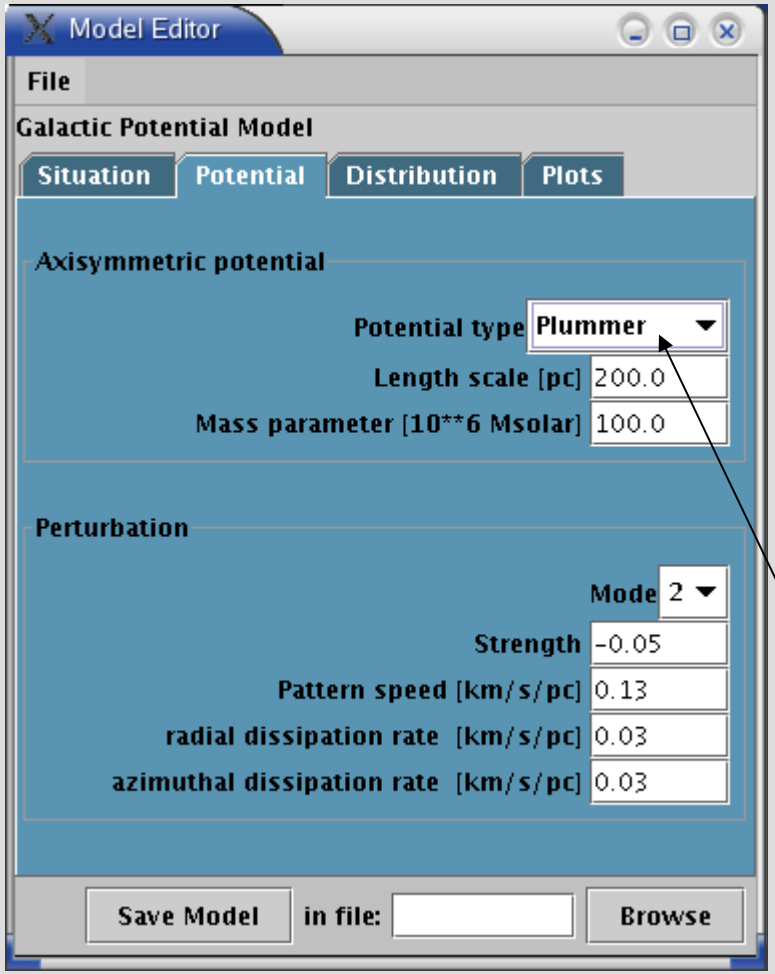
- Create a model instance (first guess)

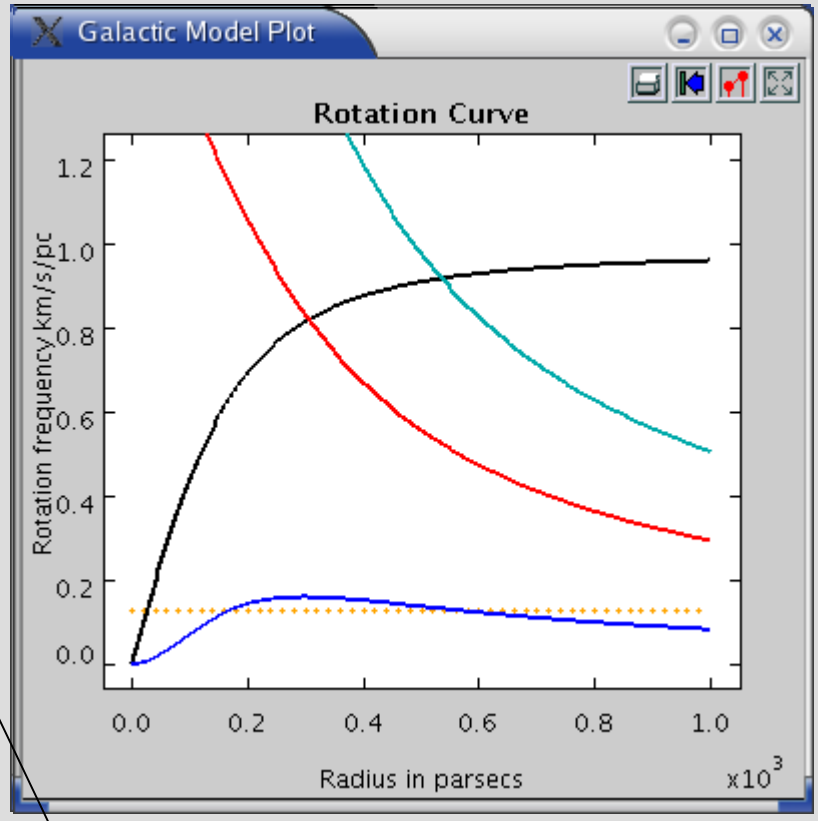


DALIA

- Create a model instance of a galactic model

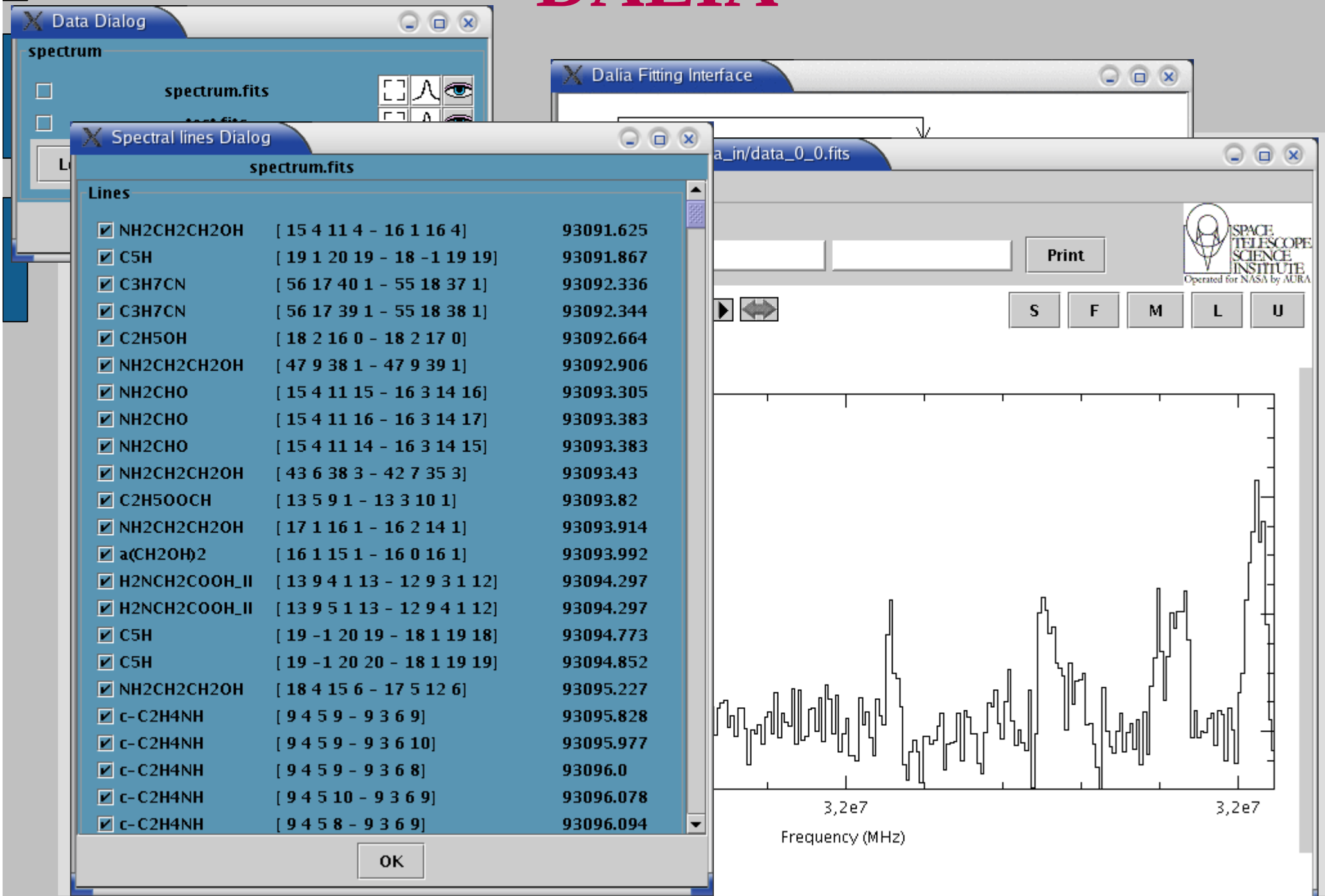
  GUI generated by the XML description of the model



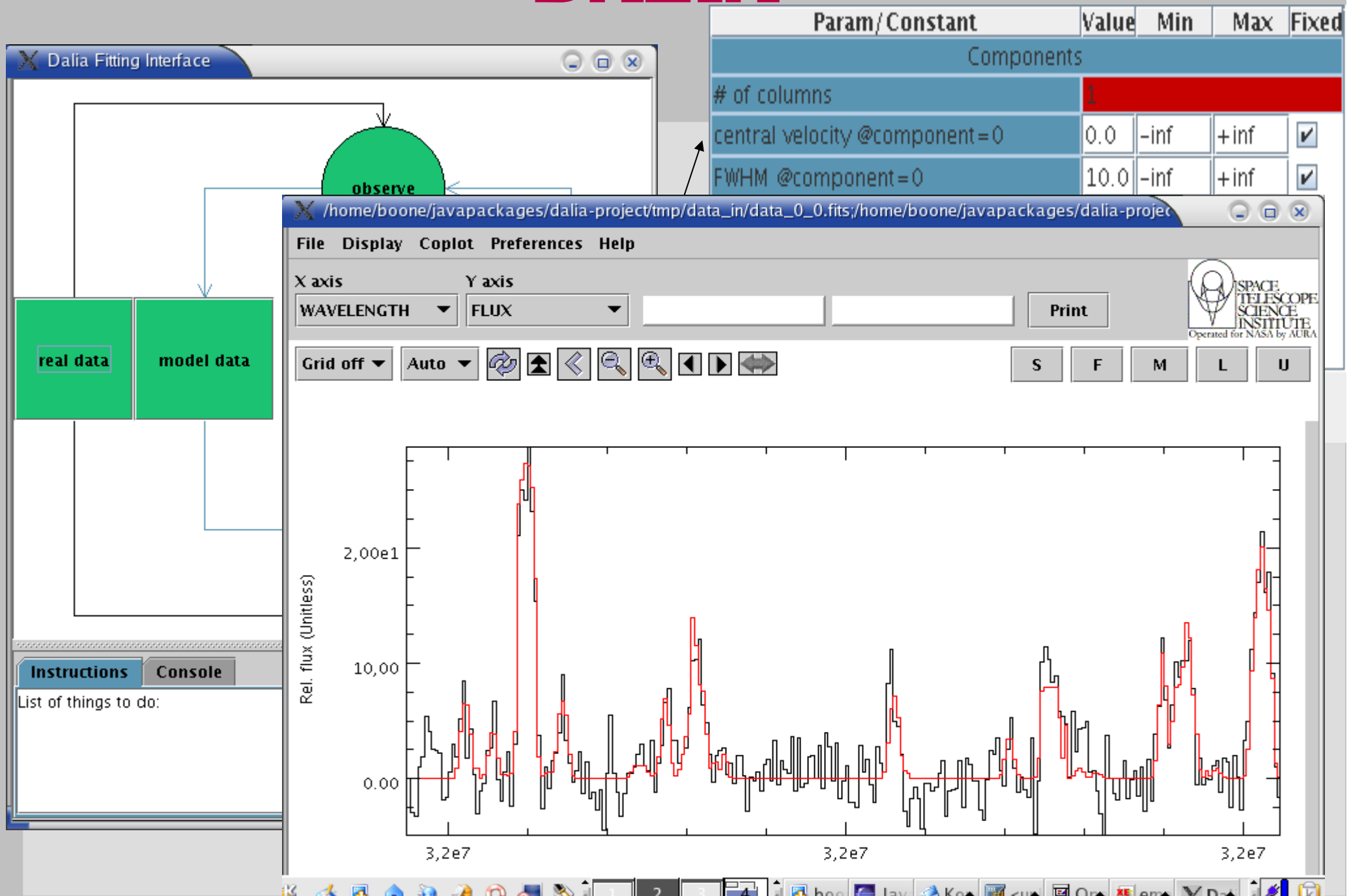


Choices

DALIA

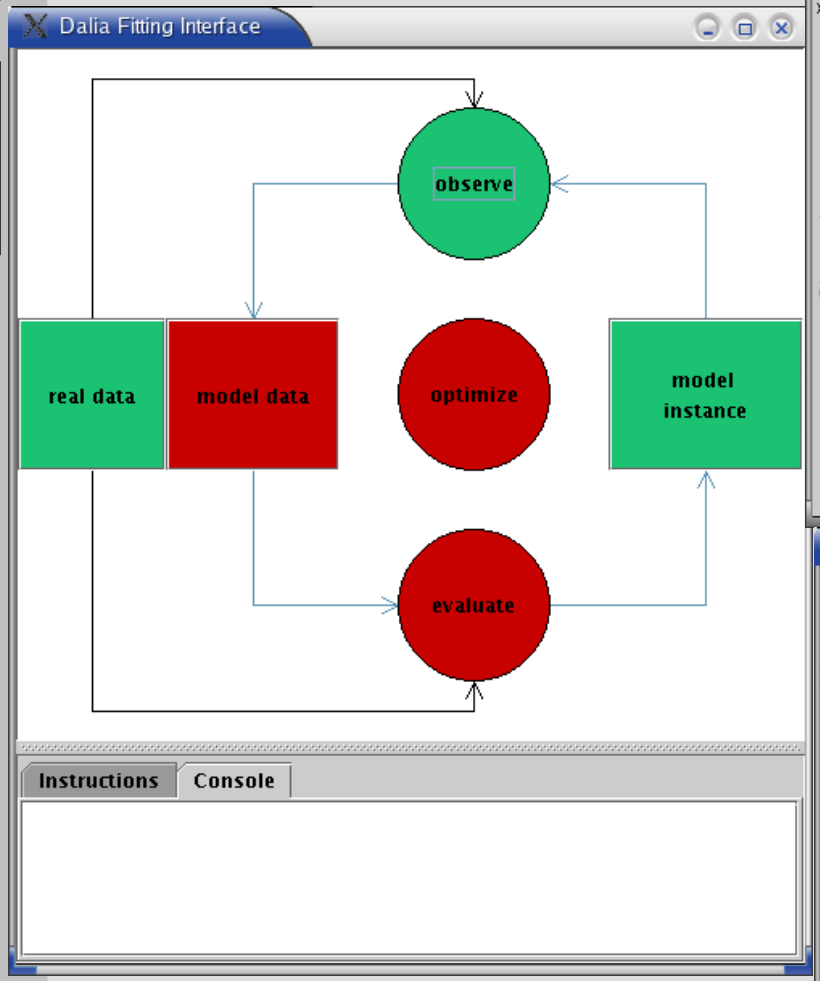

Data Dialog
spectrum
spectrum.fits
Dalia Fitting Interface
Spectral lines Dialog
spectrum.fits
Lines
NH2CH2CH2OH [15 4 11 4 - 16 1 16 4] 93091.625
C5H [19 1 20 19 - 18 -1 19 19] 93091.867
C3H7CN [56 17 40 1 - 55 18 37 1] 93092.336
C3H7CN [56 17 39 1 - 55 18 38 1] 93092.344
C2H5OH [18 2 16 0 - 18 2 17 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
a_in/data_0_0.fits
Print
SPACE TELESCOPE SCIENCE INSTITUTE
Operated for NASA by AURA
S
F
M
L
U
3,2e7
3,2e7
Frequency (MHz)

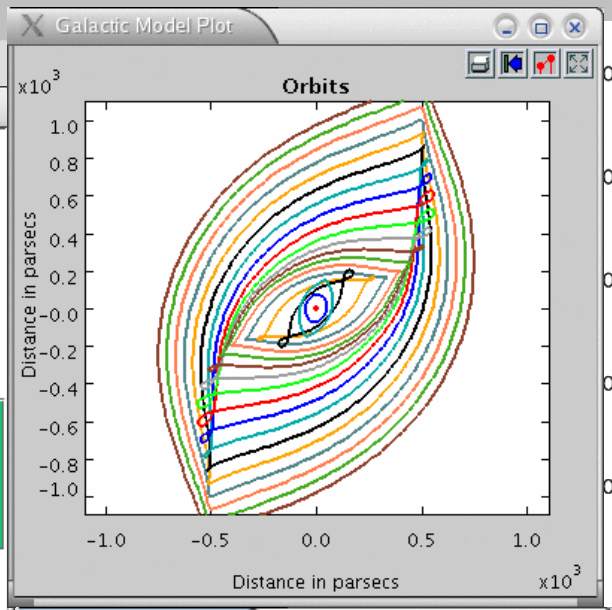
DALIA

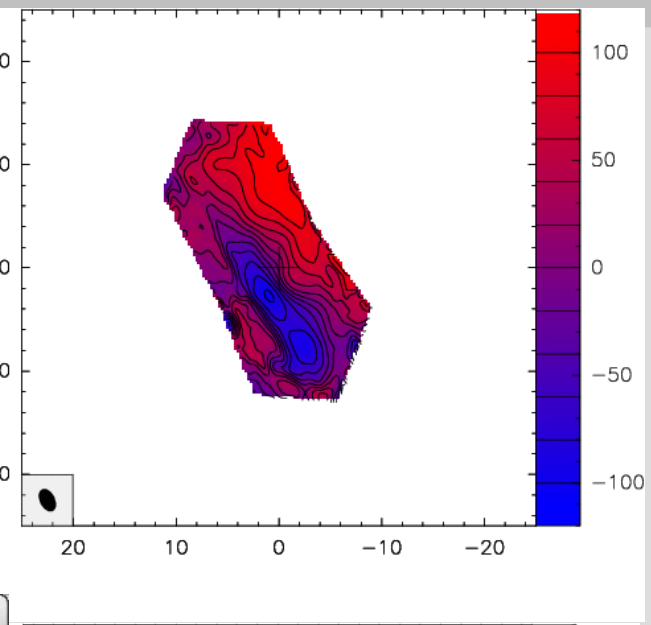

Dalia Fitting Interface
observe
real data
model data
Instructions
Console
List of things to do:
Param/Constant
Value
Min
Max
Fixed
Components
# of columns
1
central velocity @component=0
0.0
-inf
+inf
FWHM @component=0
10.0
-inf
+inf
/home/boone/javapackages/dalia-project/tmp/data_in/data_0_0.fits;/home/boone/javapackages/dalia-projec
File
Display
Coplot
Preferences
Help
X axis
Y axis
WAVELENGTH
FLUX
Print
SPACE TELESCOPE SCIENCE INSTITUTE
Operated for NASA by AURA
Grid off
Auto
S
F
M
L
U
Rel. flux (Unitless)
2,00e1
10,00
0.00
3,2e7
3,2e7
3,2e7

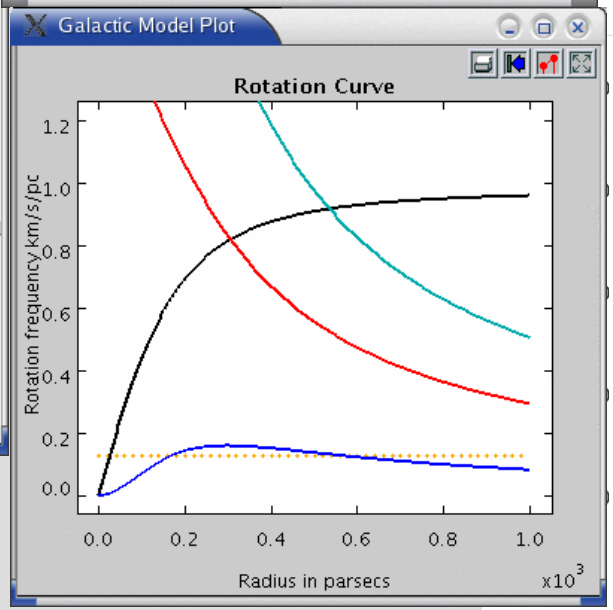
DALIA

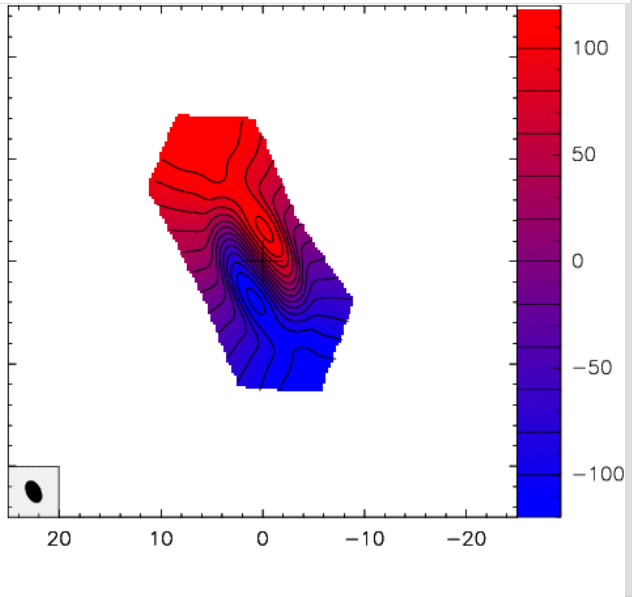
NGC 4569







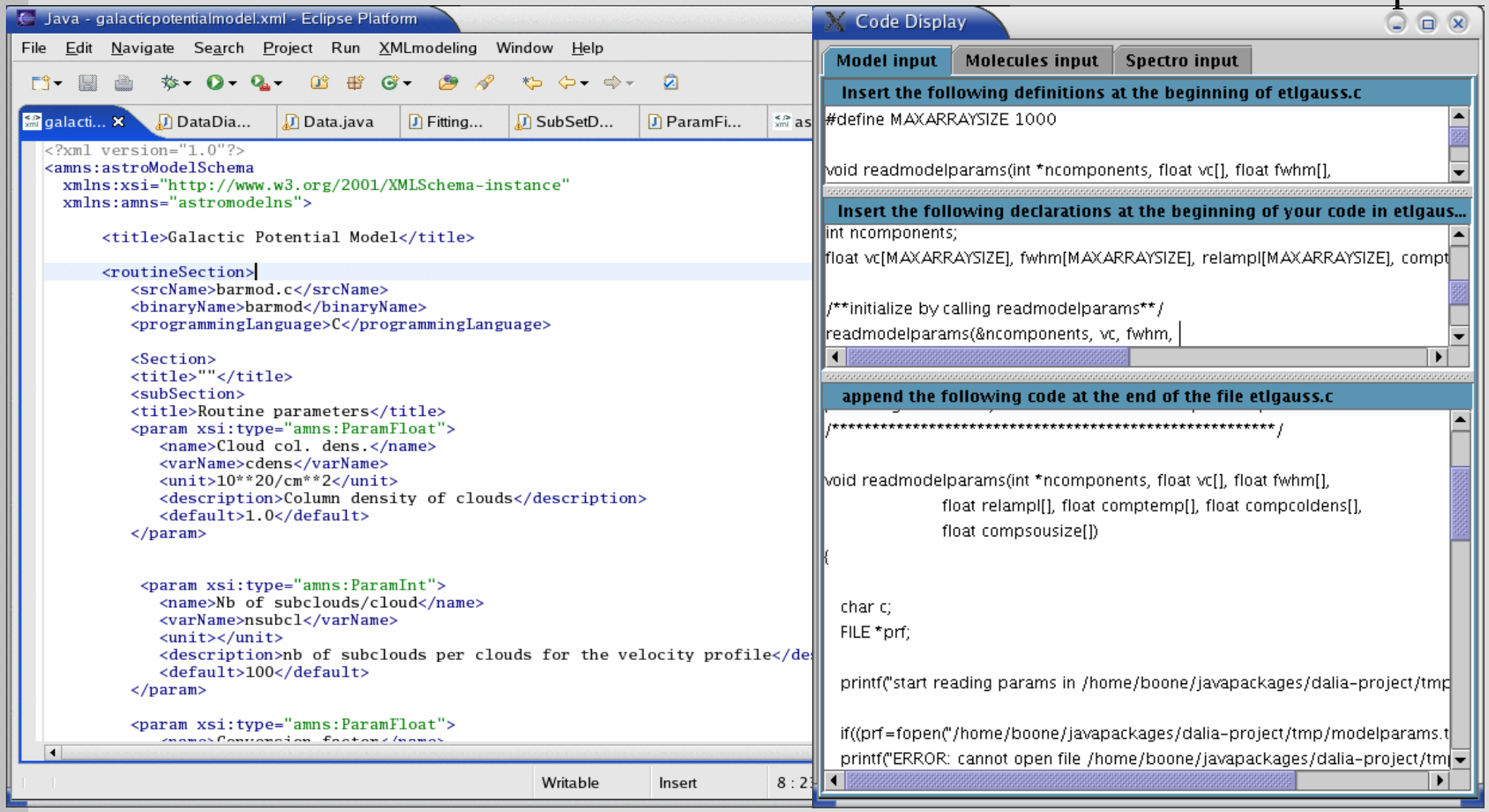




DALIA

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”**
- **Development open to the community**
- **Extensions**
  - Association with computing resources: parallel computing
  - Association with archive facilities (VO) for the data
  - Workflows (VO)