MAGIX
A Generic Framework for Science Analysis and Modelling

Frédéric Boone (Obs. Paris)
Peter Schilke (MPIfR)
Marie-Lise Dubernet (Obs. Paris)
Dirk Muders (MPIfR)
Nicolas Moreau (Obs. Paris)
Claudia Comito (MPIfR)
Silvia Leurini (ESO)
Mireille Louys (Obs. Strasbourg)
François Bonnarel (Obs. Strasbourg)

PURPOSE

Share simulation codes

--> Standards, Database

Provide tools (interfaces) to use those codes

--> Execute codes (e.g. Monte Carlo simulations)

--> Fit output to observations

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Prototype DALIA

MOTIVATIONS FOR A GENERIC INTERFACE

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

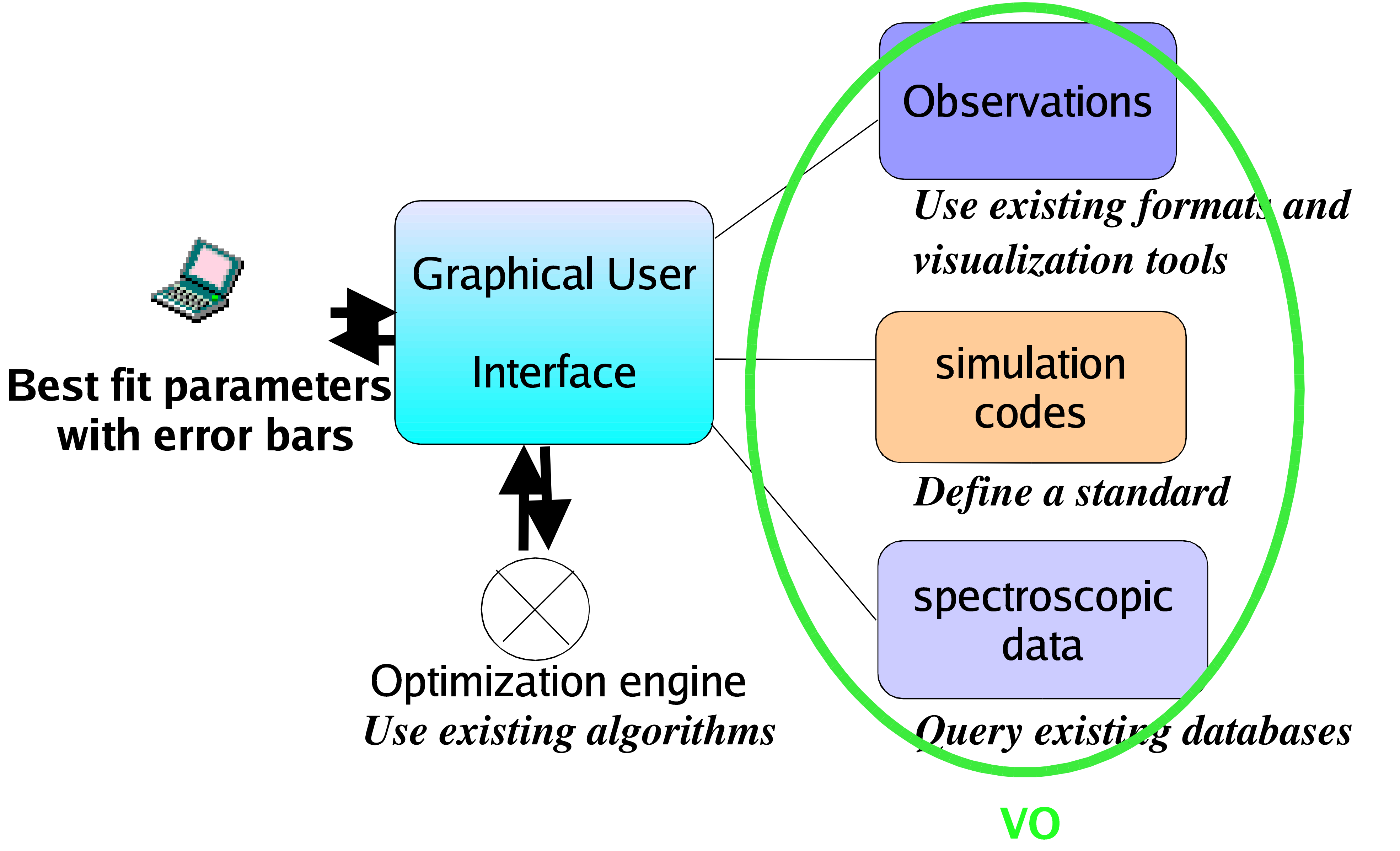
Common needs

Optimization loop to fit the model to the data with **constraints** and error estimation

Interactivity (control the model parameters)

Spectroscopic data --> query spectro databases

A GENERIC INTERFACE FOR MODELIZATION



THE PROTOTYPE, DALIA

Main functionalities

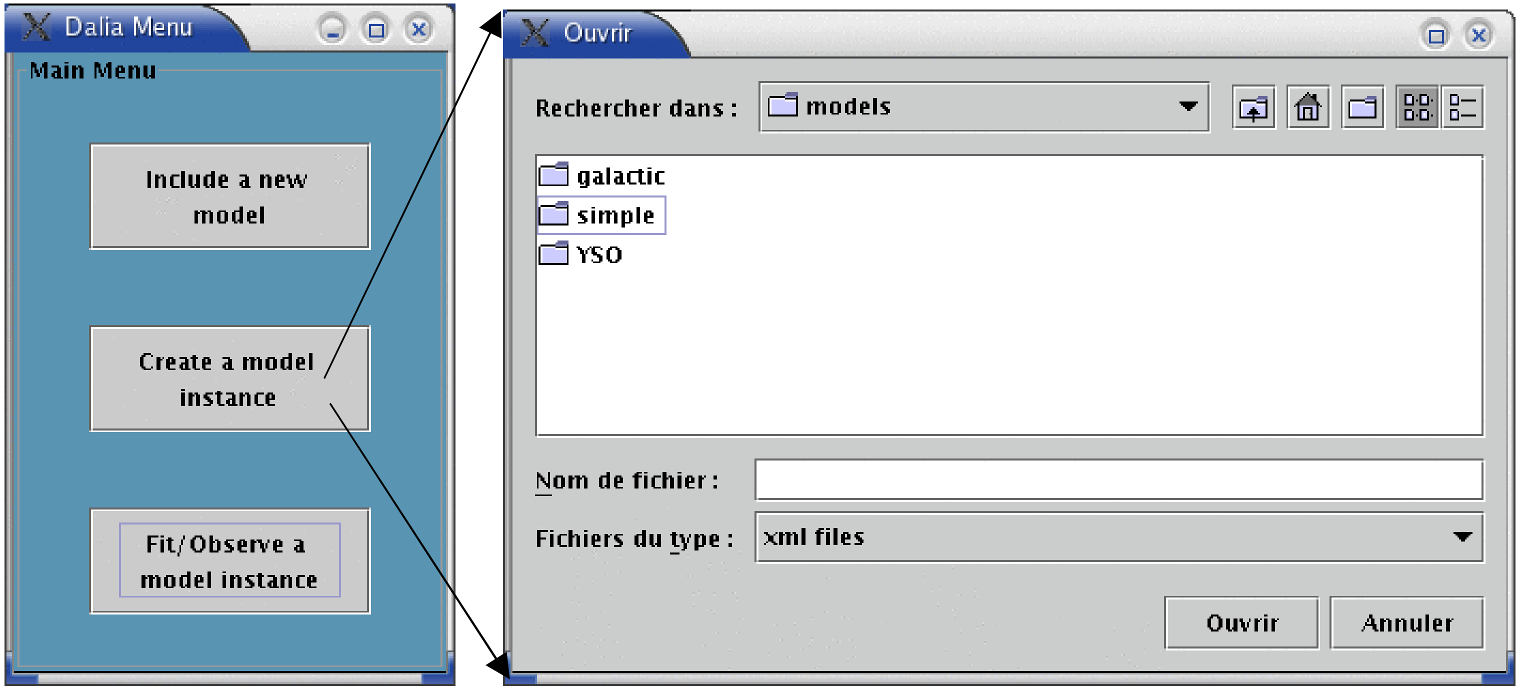
- Edit parameters of a model to create a first guess
- Fit the model to the data (1D, 2D, 3D ....) via optimization
- Constrain the parameters
- Include spectroscopic data from molecular databases
- Allow to introduce any new model code (Fortran, C...)

Implementation

- GUI in JAVA
- Description of simulation codes in XML following a “schema”
- Interface GUI/models: ASCII for params and FITS for data
- Visualization: Specview (spectra) imageJ (2d & 3d)

DALIA

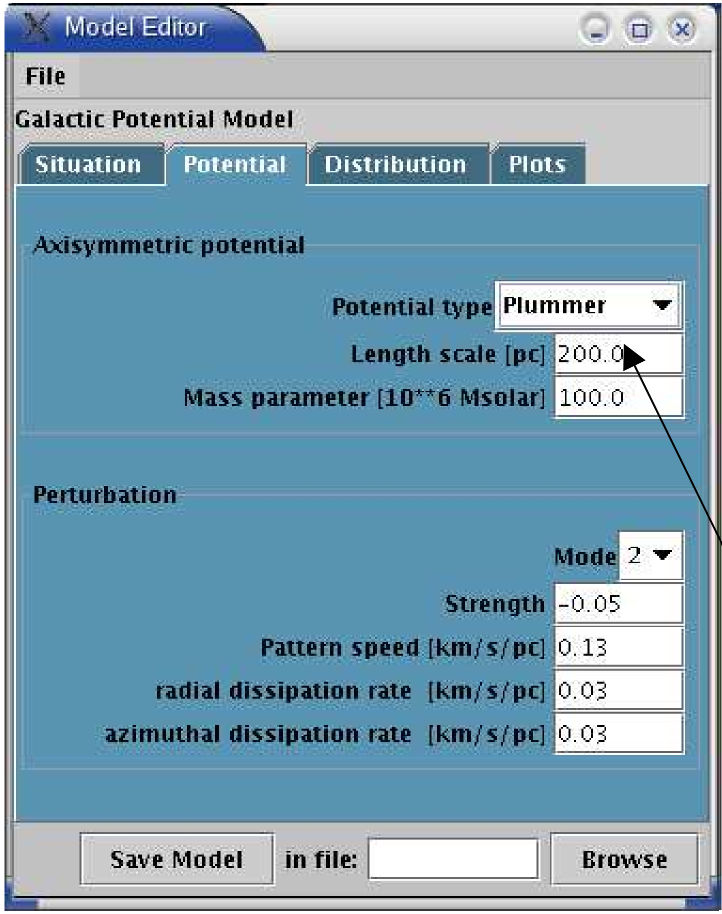
Create a model instance (first guess)

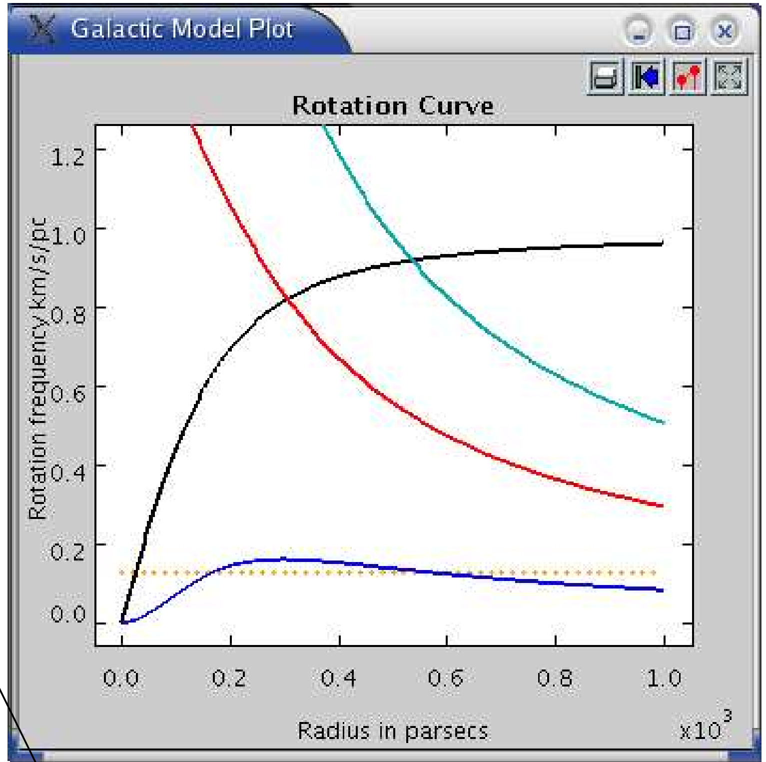


DALIA

- Create a model instance of a galactic model

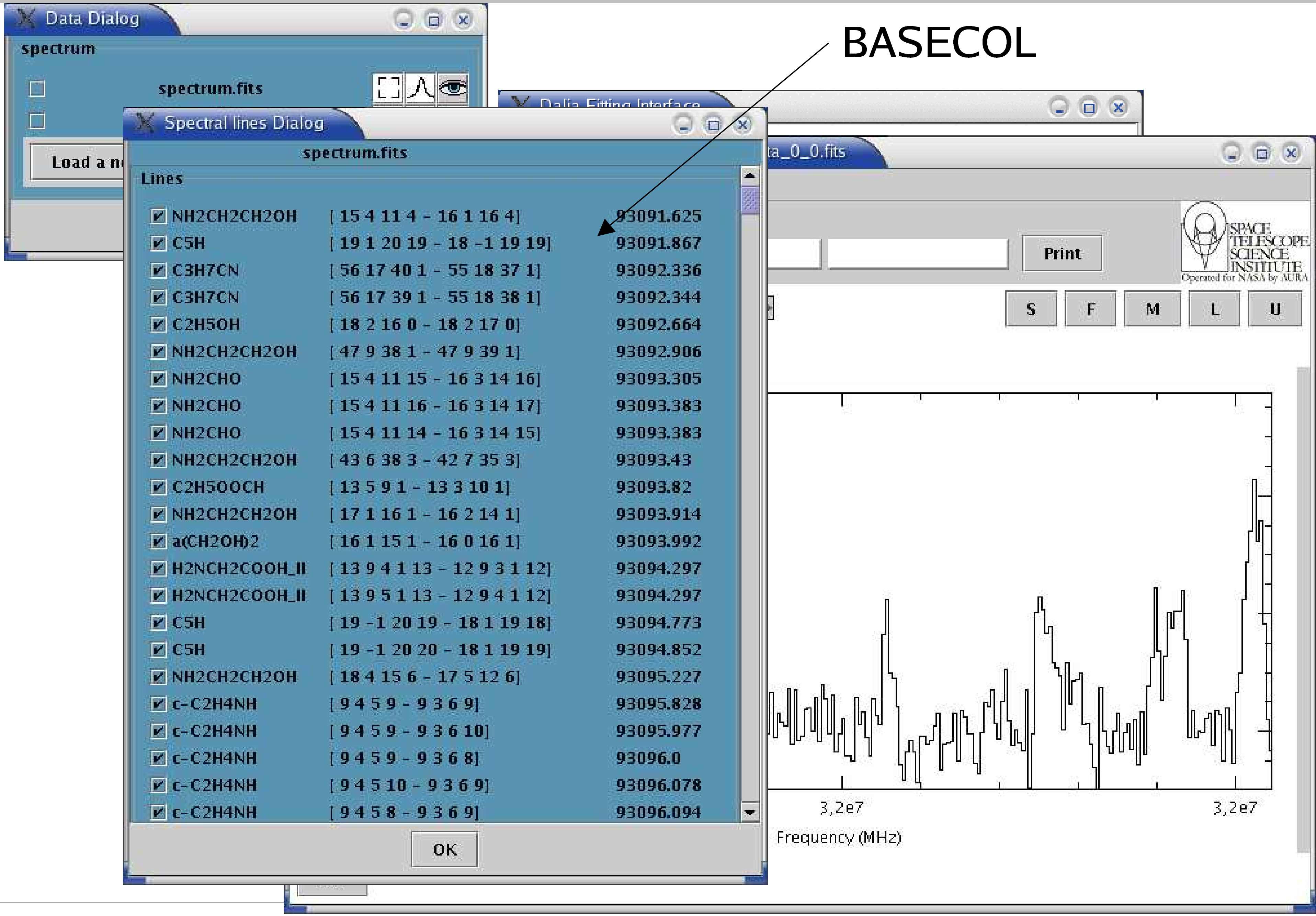
GUI generated by the XML description of the simulation code



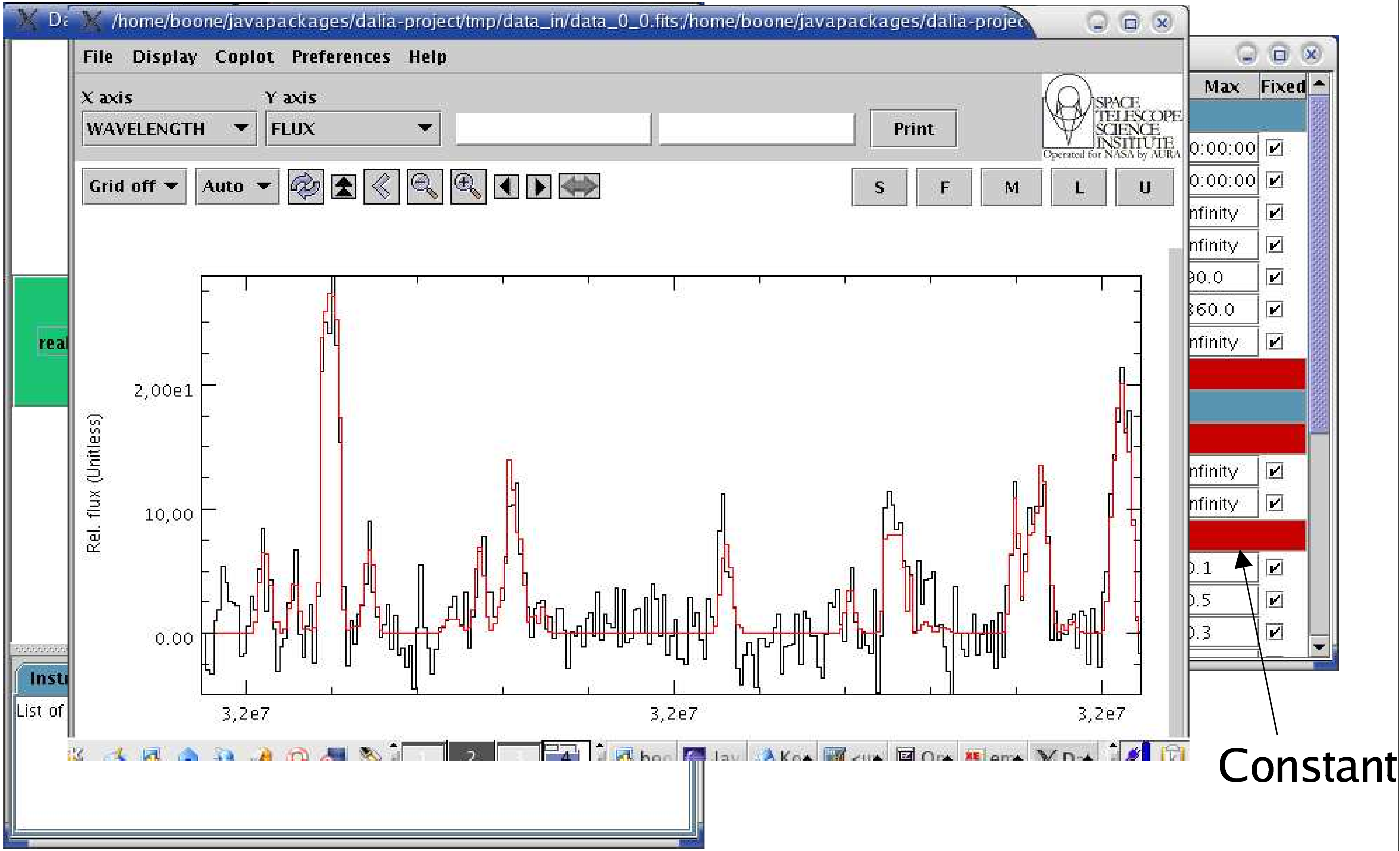


Choices

DALIA

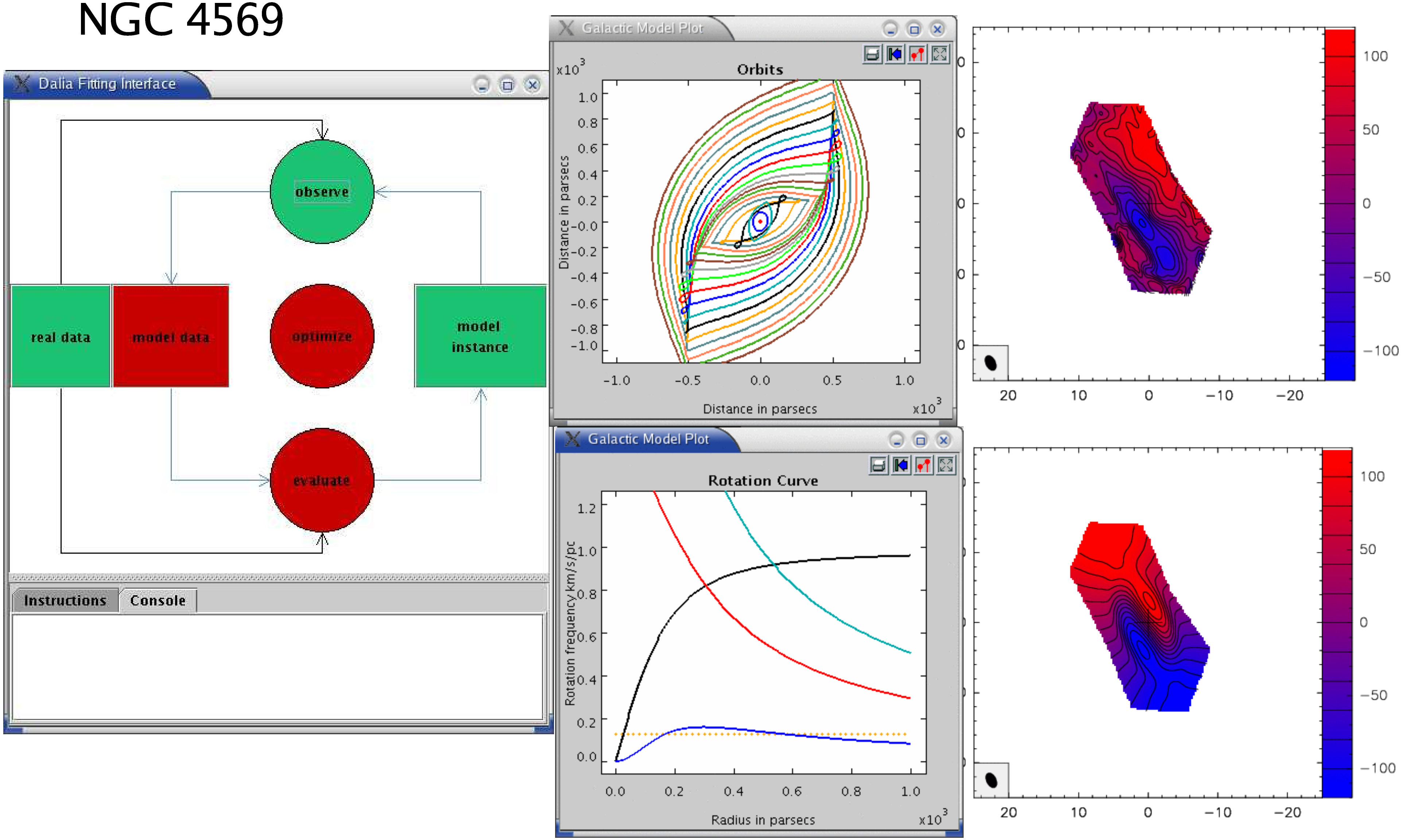

BASECOL
Data Dialog
spectrum
spectrum.fits
Load a n
Dalia Fitting Interface
ta_0_0.fits
Print
SPACE TELESCOPE SCIENCE INSTITUTE
Operated for NASA by AURA
S
F
M
L
U
3,2e7
3,2e7
Frequency (MHz)
Spectral lines Dialog
spectrum.fits
Lines
NH2CH2CH2OH [15 4 11 4 - 16 1 16 4] 93091.625
C5H [19 1 20 19 - 18 -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

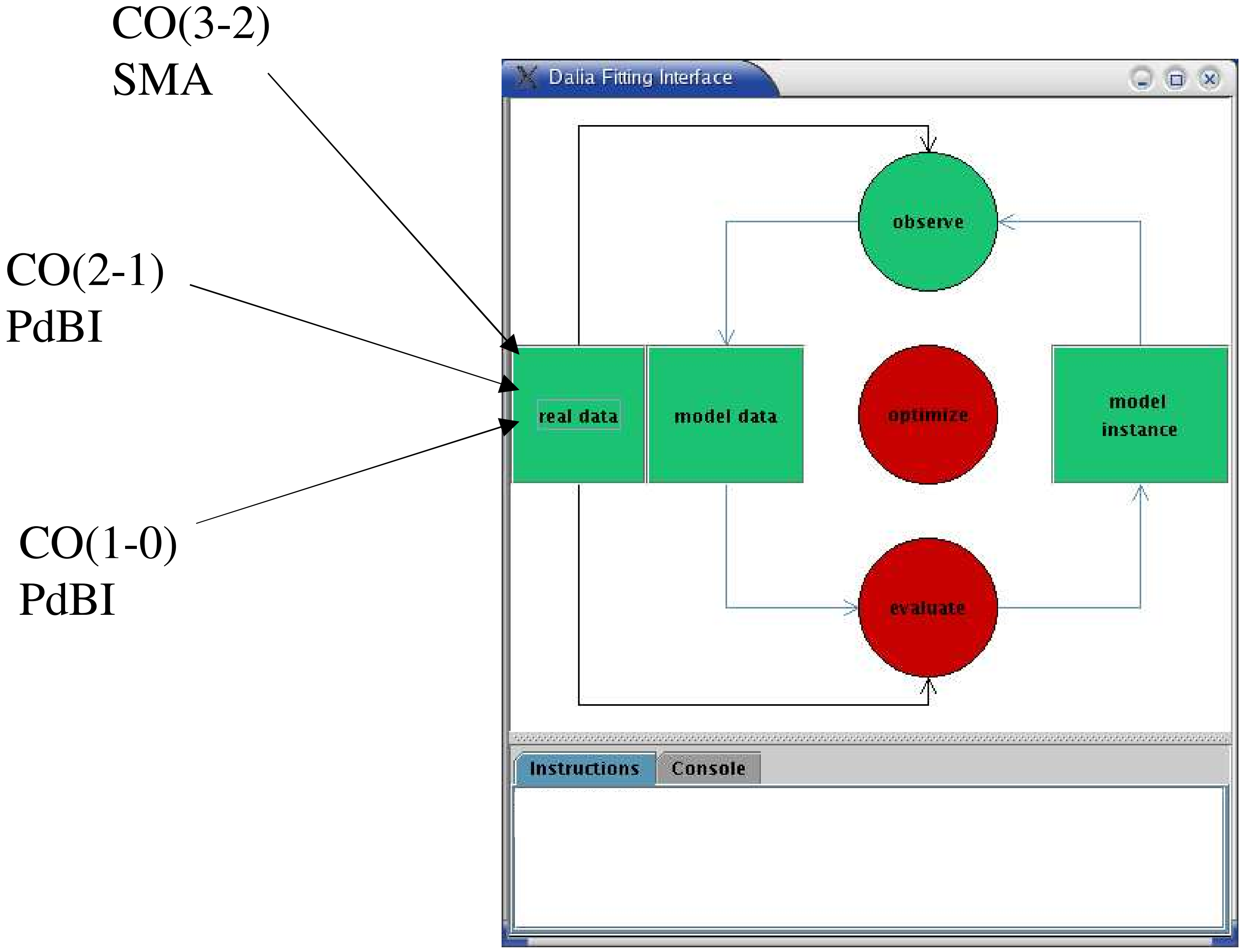
DALIA


/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
Max
Fixed
Constant

DALIA

NGC 4569




CO(3-2)
SMA
CO(2-1)
PdBI
CO(1-0)
PdBI
Dalia Fitting Interface
observe
real data
model data
optimize
model
instance
evaluate
Instructions
Console

PURPOSE

Share simulation codes

--> Standards, Database

IVOA standard

Provide tools (interfaces) to use those codes

--> Execute codes (e.g. Monte Carlo simulations)

--> Fit output to observations

MOTIVATIONS FOR SHARING SIMULATION CODES

Same motivation as for data sharing

Allow multiwavelength and large number statistics

--> multiwavelength and “multi-physics” analysis

Check published results

--> reproductibility of theoretical models

Rewarding for instrument developers

--> rewarding for code publishers

+ required by data sharing

Many different physical processes covered by data

CHALLENGES

Same as for data sharing

- Some don't like to share data with other teams (a few only)
- --> some do not like to share their code (great majority!)
- Data can be misinterpreted by non-specialists ("dangerous")
- --> simulation codes can be misused by non-specialists
- Need to define standards

Additional problems specific to codes

- Need to define 2 standards: code description AND protocol
- Binaries can not be standard: portability

Different types of information required

- Inputs related to the *astrophysical source*

  inclination, size of disk etc...

- Inputs related to *instrumental effects*

  psf, etc ...

- Inputs related to the *algorithm* used in the code

  number of particles

--> **New data model for parameter sets**

- Inputs related to general *knowledge in physics*

  frequency(ies) of the transition(s) considered (Halpha or CO etc...) for the emission

--> **Point to Atomic Line data model (e.g. Dubernet et al)**

- Output dataset(s)

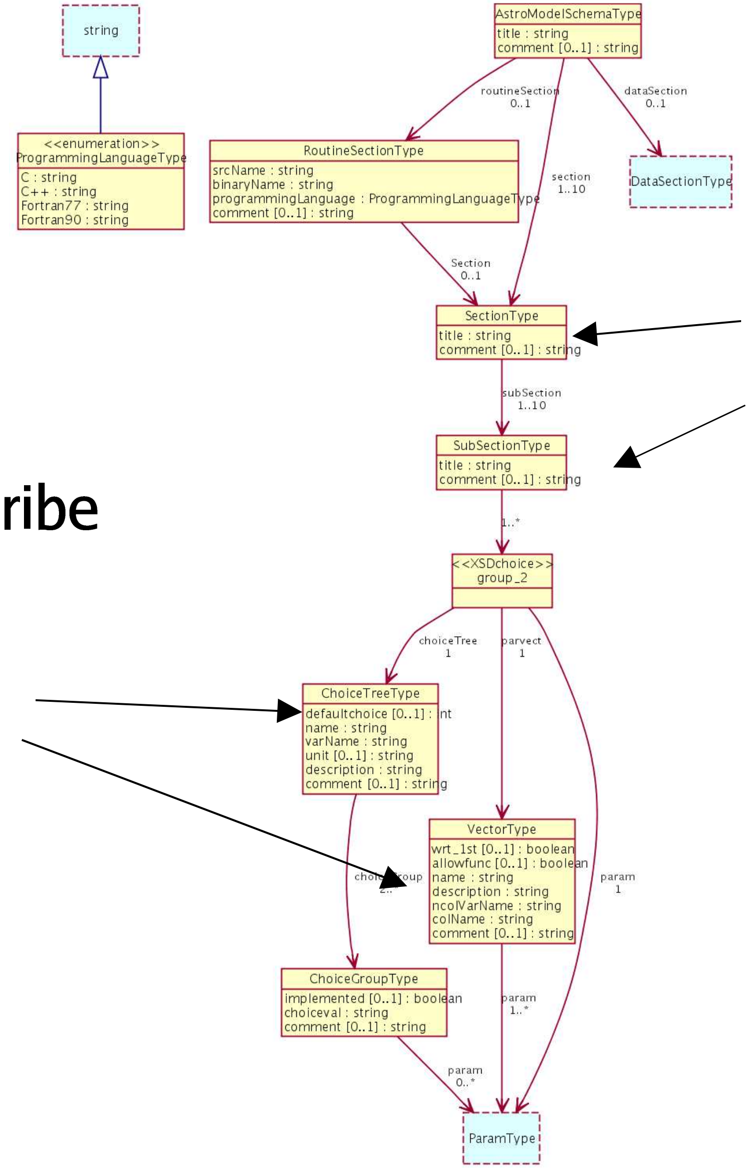
  number of axes, nature of axes, ...

--> **Point to Characterisation, Spectrum data models**

Parameter Model Requirements

- To **structure** the parameter set (Sections, Subsections...)
  --> The code provider may structure the parameters according to their physical meaning to help the user to catch the physics behind
- Allow for **dynamical** description
  - Hierarchy (a parameter determines a subset of parameters)
  - Tables (several parameters can be vectors of variable length)
- Allow **information on the numerical code** (program) to be included (native language, variable names used in the code)
  --> help user/application to implement protocol for data exchange with code (generate pieces of codes in the native language)

The UML Schema



Objects to structure the description of parameter sets

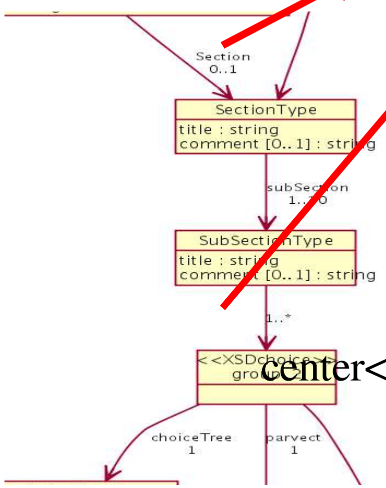
Objects to describe dynamical parameter sets

Structured parameter set

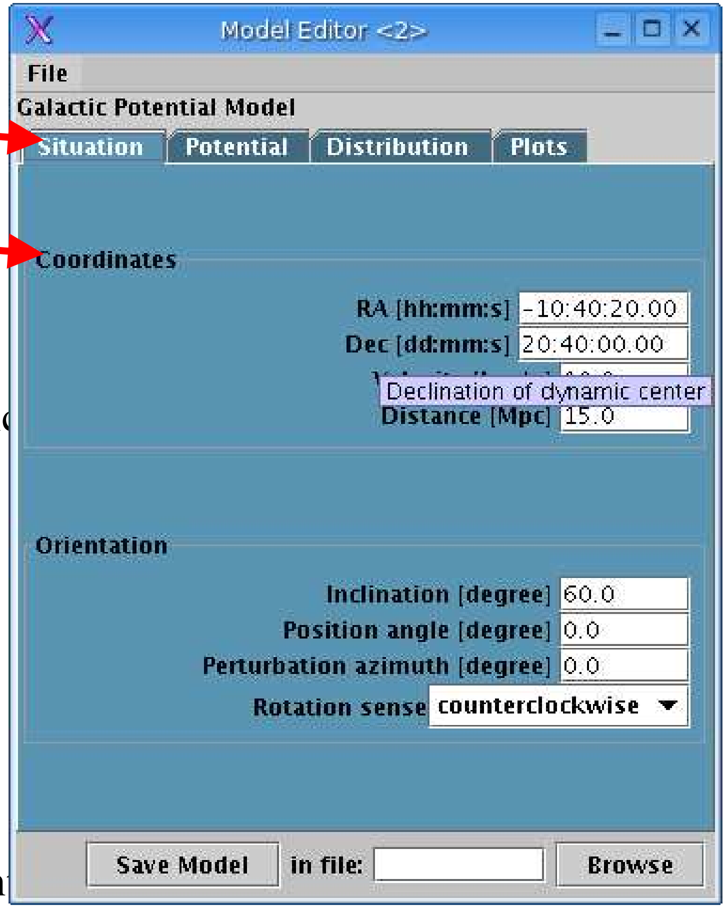
UML

XML INSTANCE

DALIA GUI

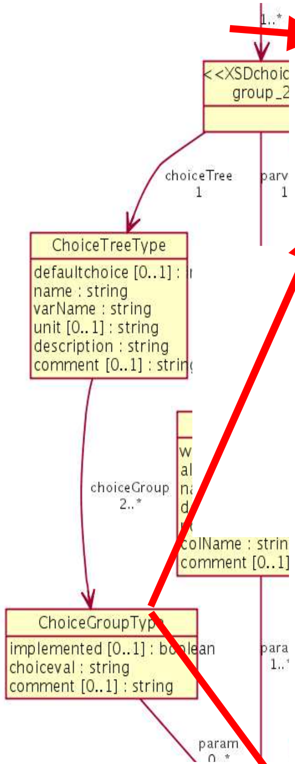



```
<section>
 <title>Situation</title>
   <subSection>
     <title>Coordinates</title>

      <param xsi:type="amns:ParamCoor">
        <name>RA</name>
        <varName>ra</varName>
        <unit>hh:mm:s</unit>
        <description>Right Ascension of dynamic
center</description>
        <default>-10:40:20.00</default>
      < /param>

      <param xsi:type="amns:ParamCoor">
        <name>Dec</name>
        <varName>dec</varName>
        <unit>dd:mm:s</unit>
        <description>Declination of dynamic cen
        <default>20:40:00.00</default>
      </param>
```

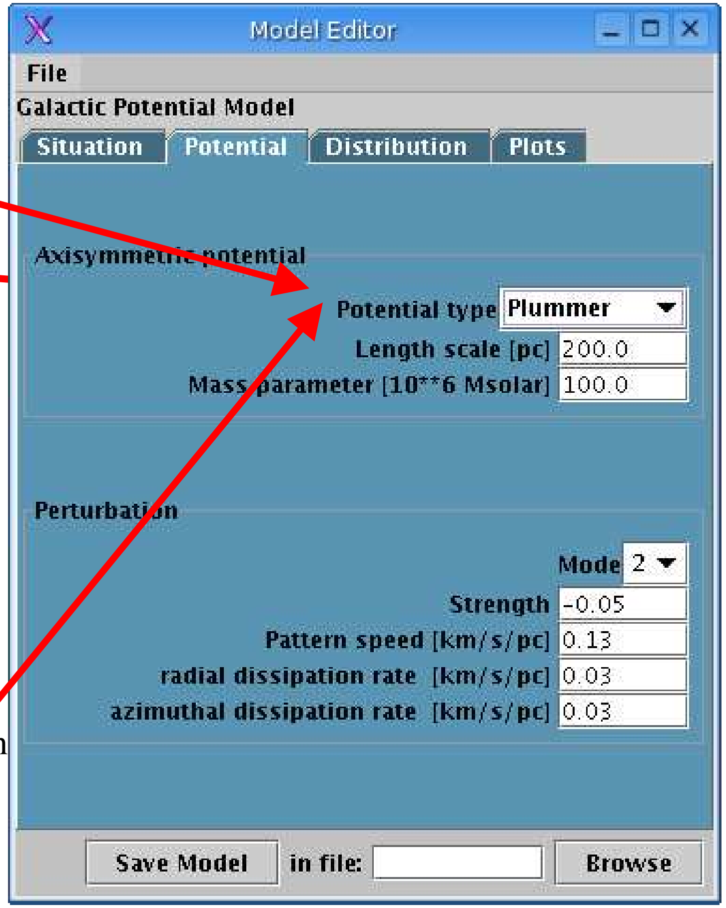


Hierarchy in a dynamical parameter set

UML | XML INSTANCE | DALIA GUI

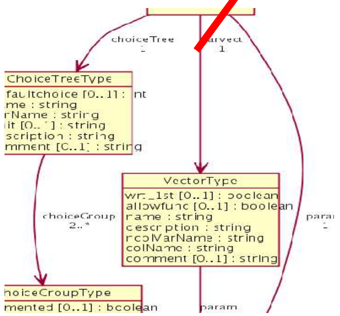



```xml
<choiceTree>
<name>Potential type</name>
<varName>pottype</varName>
<description>Potential shape</description>
<choiceGroup>
  <choiceval>Logarithmic</choiceval>
  <param xsi:type="amns:ParamFloat">
    <name> Length scale </name>
    <varName>rp</varName>
    <unit>pc</unit>
    <description>Length scale of potential</description>
    <default>200</default>
  </param>
  <param xsi:type="amns:ParamFloat">
    <name>Velocity scale</name>
    <varName>vp</varName>
    <unit>km/s</unit>
    <description> velocity scale of potential </description>
    <default>100</default>
  </param>
</choiceGroup>
<choiceGroup implemented="true">
  <choiceval>Plummer</choiceval>
  <param xsi:type="amns:ParamFloat">
    <name>Length scale</name>
```



Dynamical table of parameters

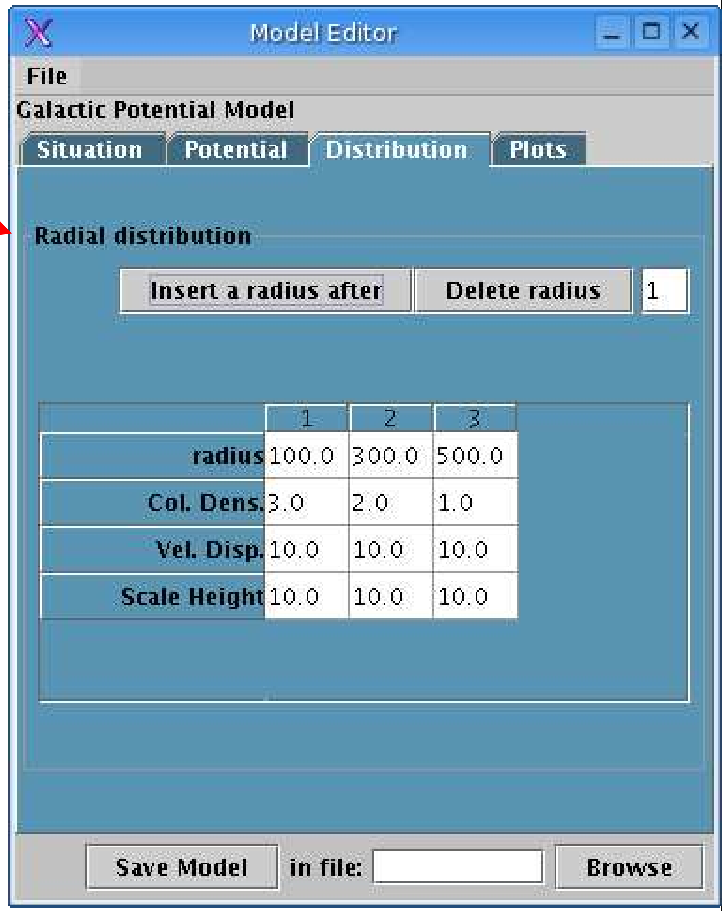
UML



XML INSTANCE

```
<parvect>
<name>Radial distribution</name>
<description>Radial distribution of matter</description>
<ncolVarName>nur</ncolVarName>
<colName>radius</colName>
  <param xsi:type="amns:ParamFloat">
    <name>radius</name>
    <varName>uradii</varName>
    <unit>pc</unit>
    <description>Radius in pc</description>
    <default>100.</default>
 </param>
 <param xsi:type="amns:ParamFloat">
    <name>Col. Dens.</name>
    <varName>udens</varName>
    <unit>10^22 cm-2</unit>
    <description>Comlumn density</description>
    <default>1.</default>
  </param>
   <param xsi:type="amns:ParamFloat">
    <name>Vel. Disp.</name>
    <varName>udisp</varName>
    <unit>km/s </unit>
    <description>Velocity dispersion </description>
    <default>10.</default>
  </param>
   <parvect>
```

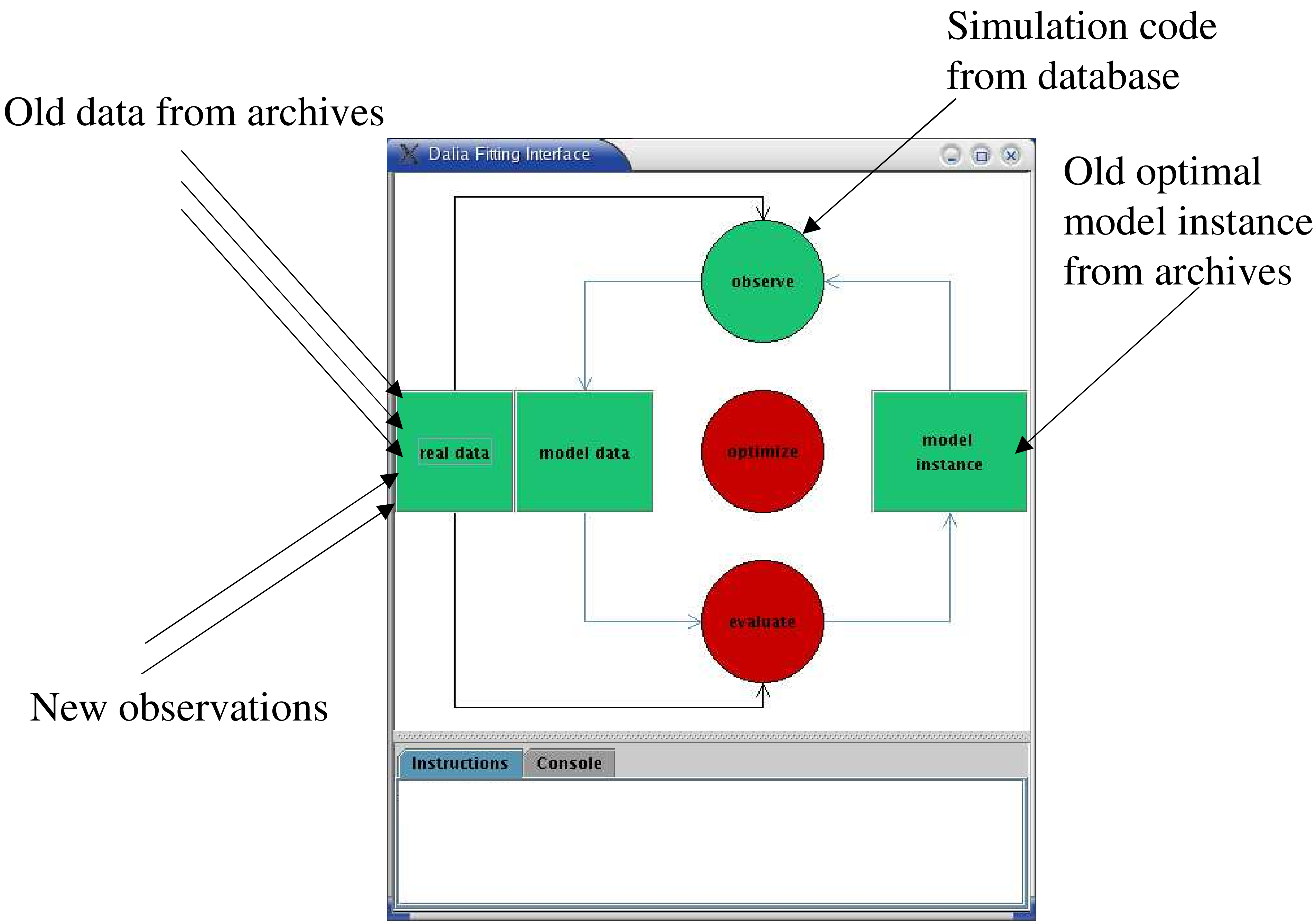
DALIA GUI



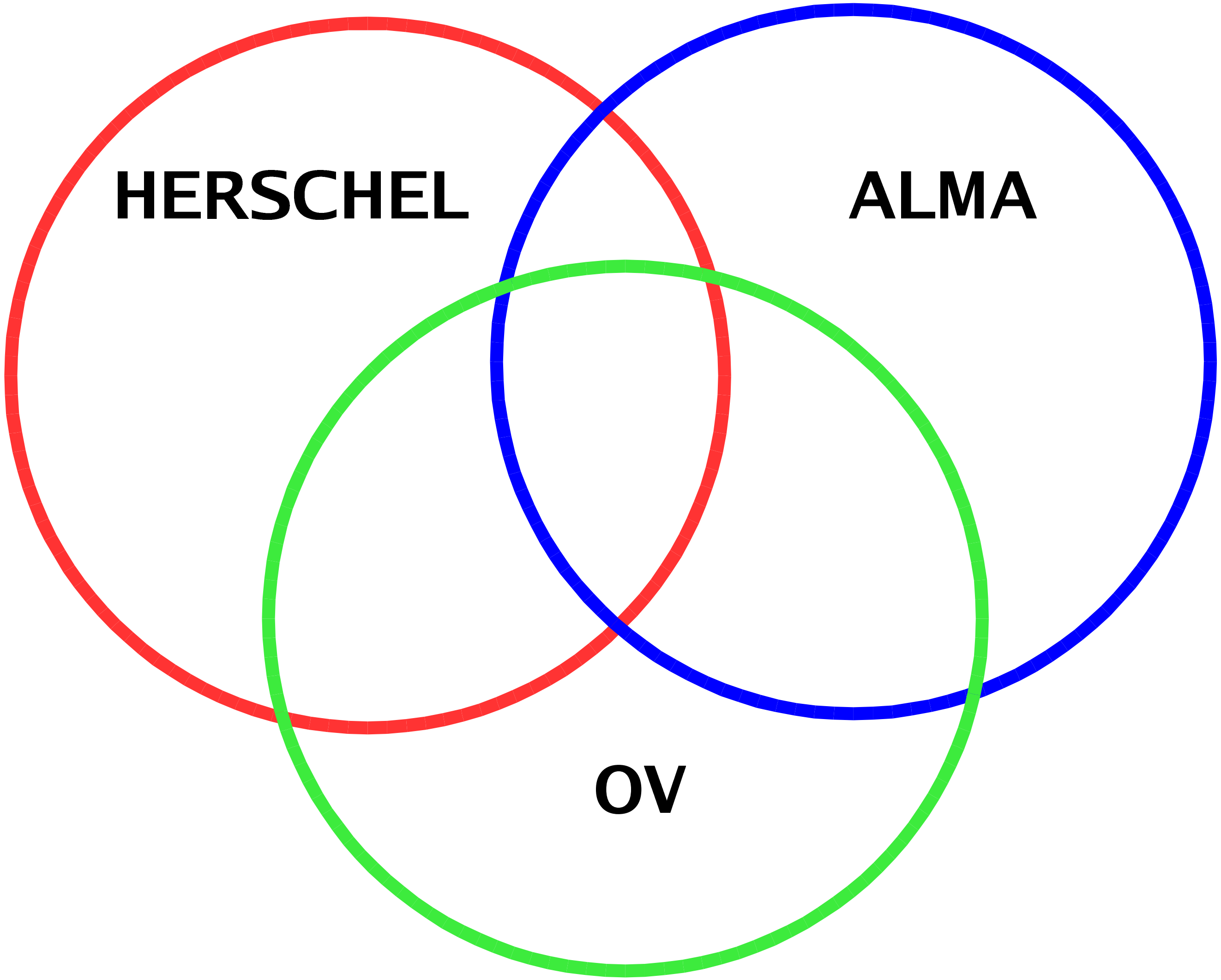
Perspectives

- Publish numerical models for data analysis through a Registry
- Share « instances » of models in the sense of an instance of parameter set:
  - e.g. result of a model fit = values of the best fit parameters --> need to define a data model for instances of parameter sets

    ==> share theoretical knowledge at the same level as the observations



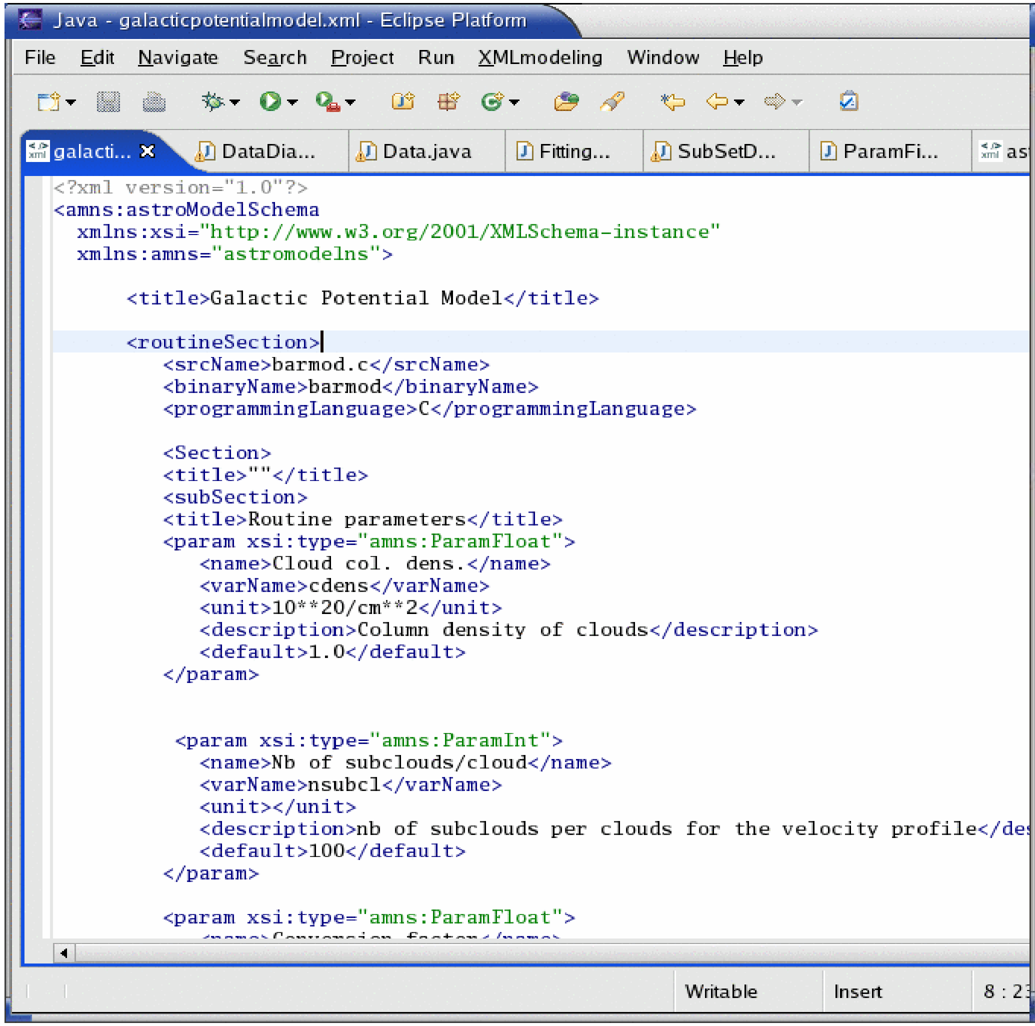
Simulation code from database
Old data from archives
Dalia Fitting Interface
Old optimal model instance from archives
observe
real data
model data
optimize
model instance
evaluate
New observations
Instructions
Console

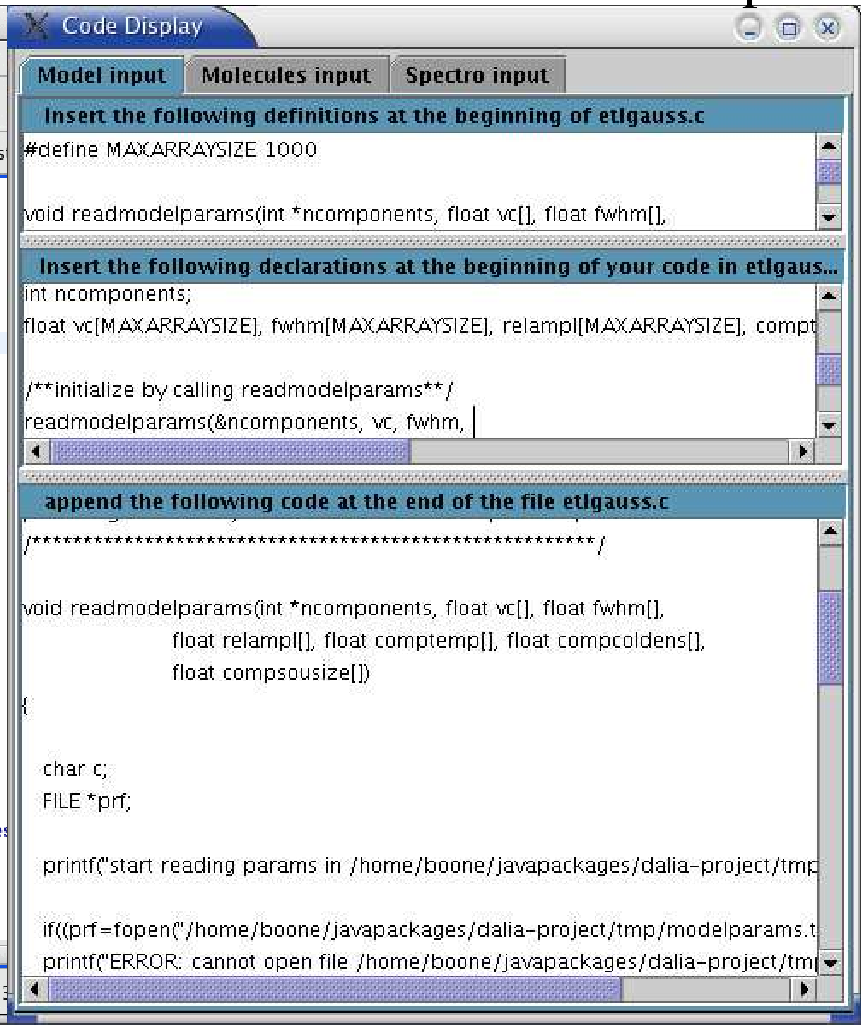

HERSCHEL
ALMA
OV

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, Not only astronomy?
- **Possible extensions**
  - Association with computing resources: server (web service), paralel computing
  - Association with archive facilities (VO) for the data but also for the model codes and the model instances

Outlook

- **Wish of the community to share models (?)**
- **Models should be well documented**
- **Development open to the community**
  MPIfR + Observatoire de Paris +Strasbourg+...

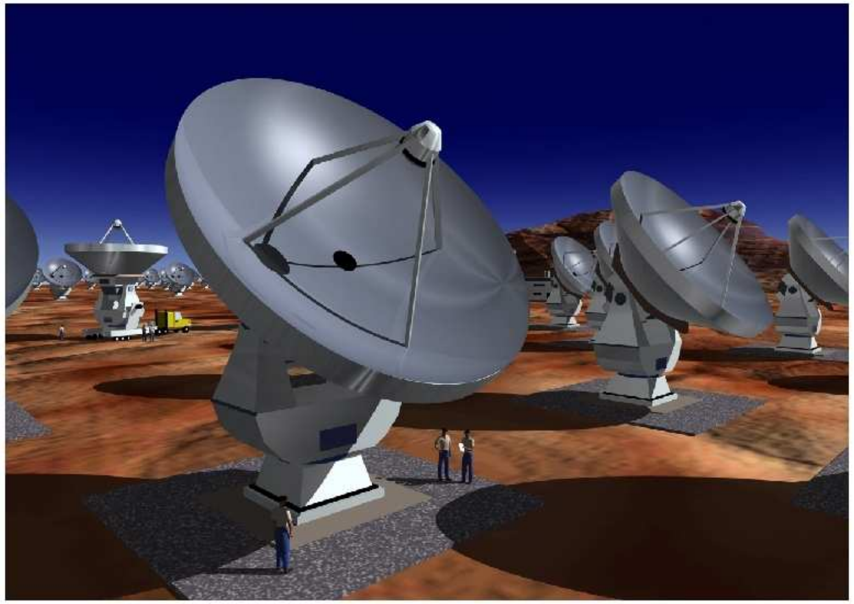
Plateau de Bure (IRAM) 6x15m λ=[1, 3] mm

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

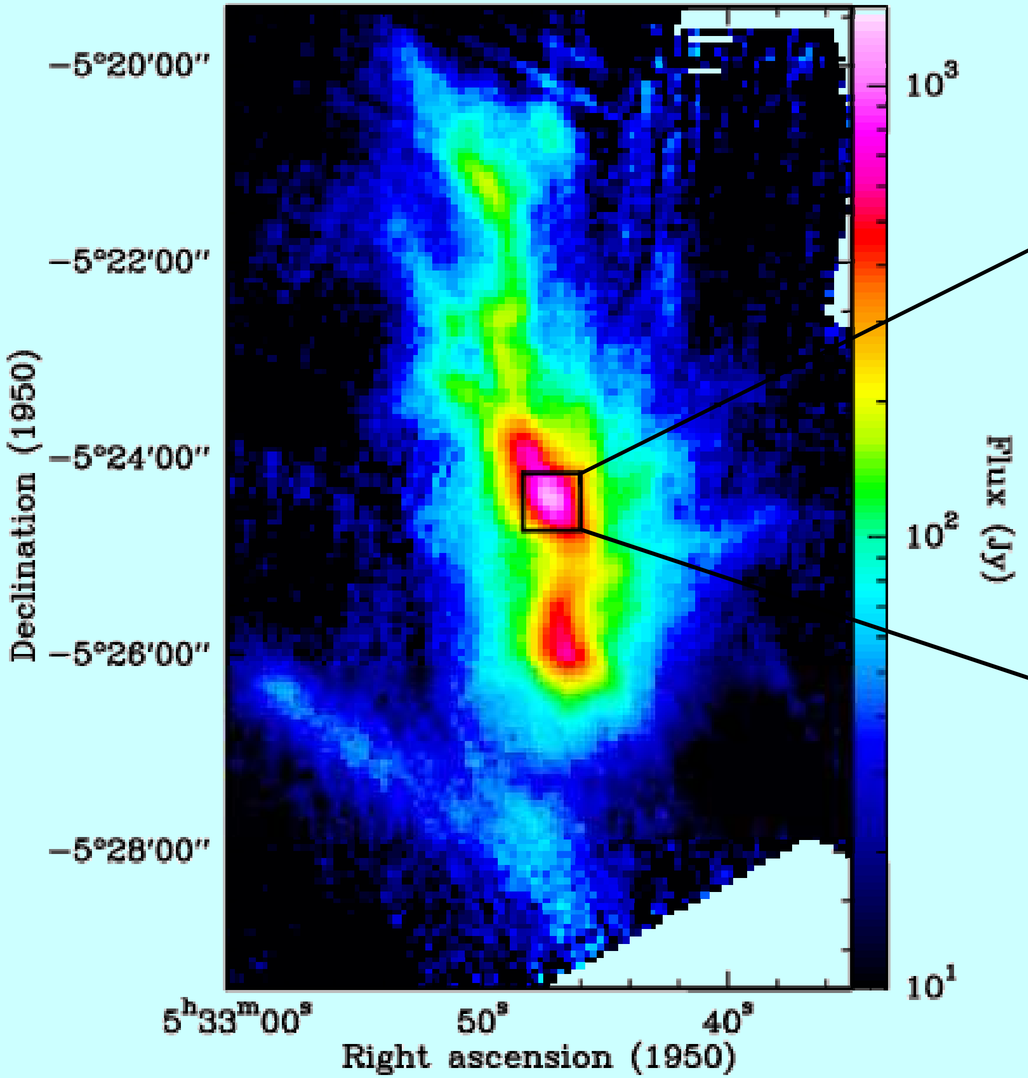


Herschel (ESA) 3.5m λ=[60, 670]mu

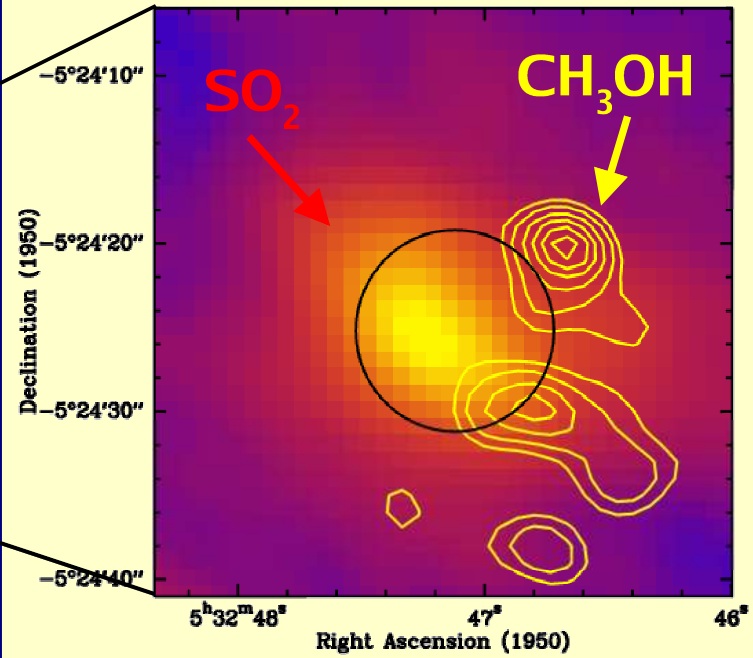
Example I – Line surveys

- **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

ORION-KL



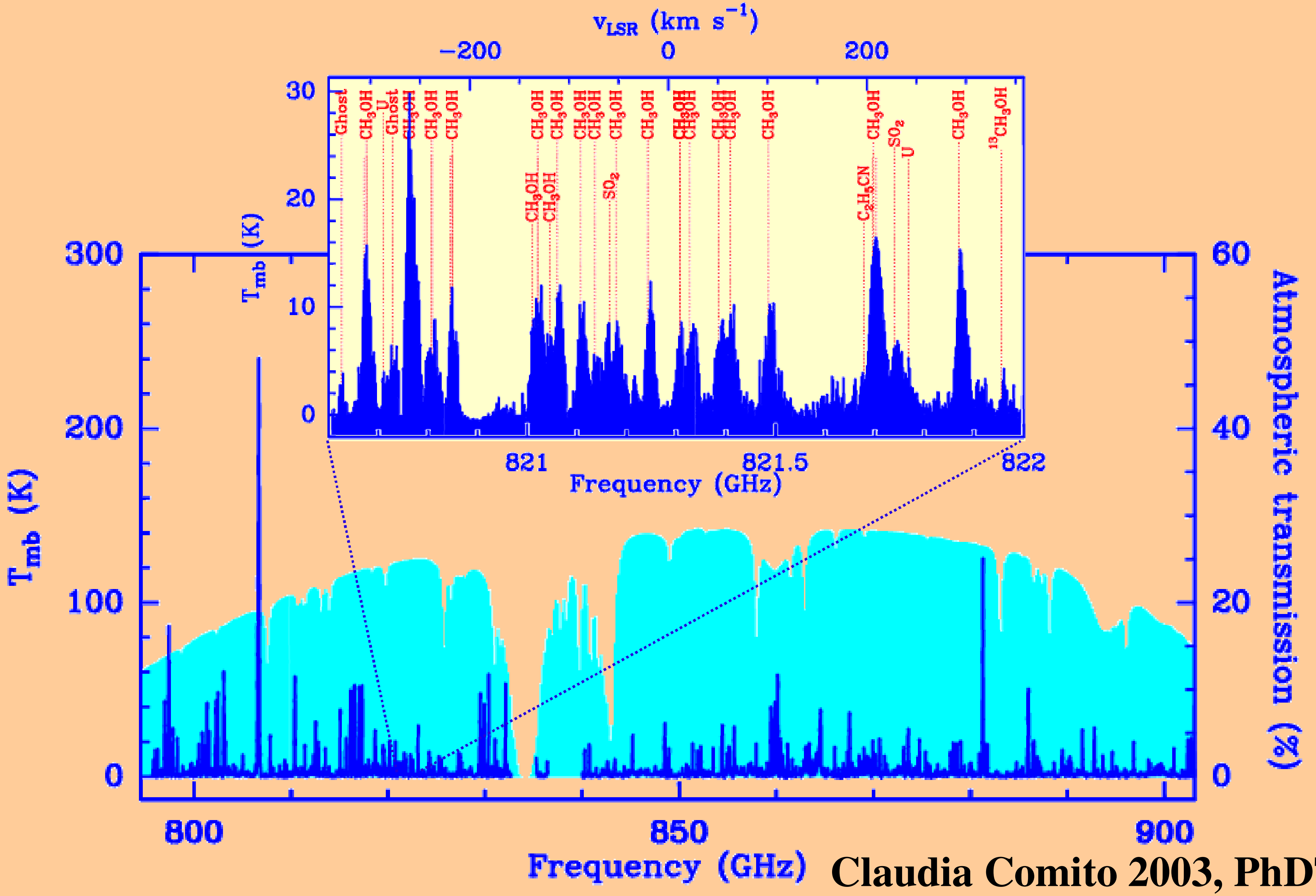
Lis et al., 1998



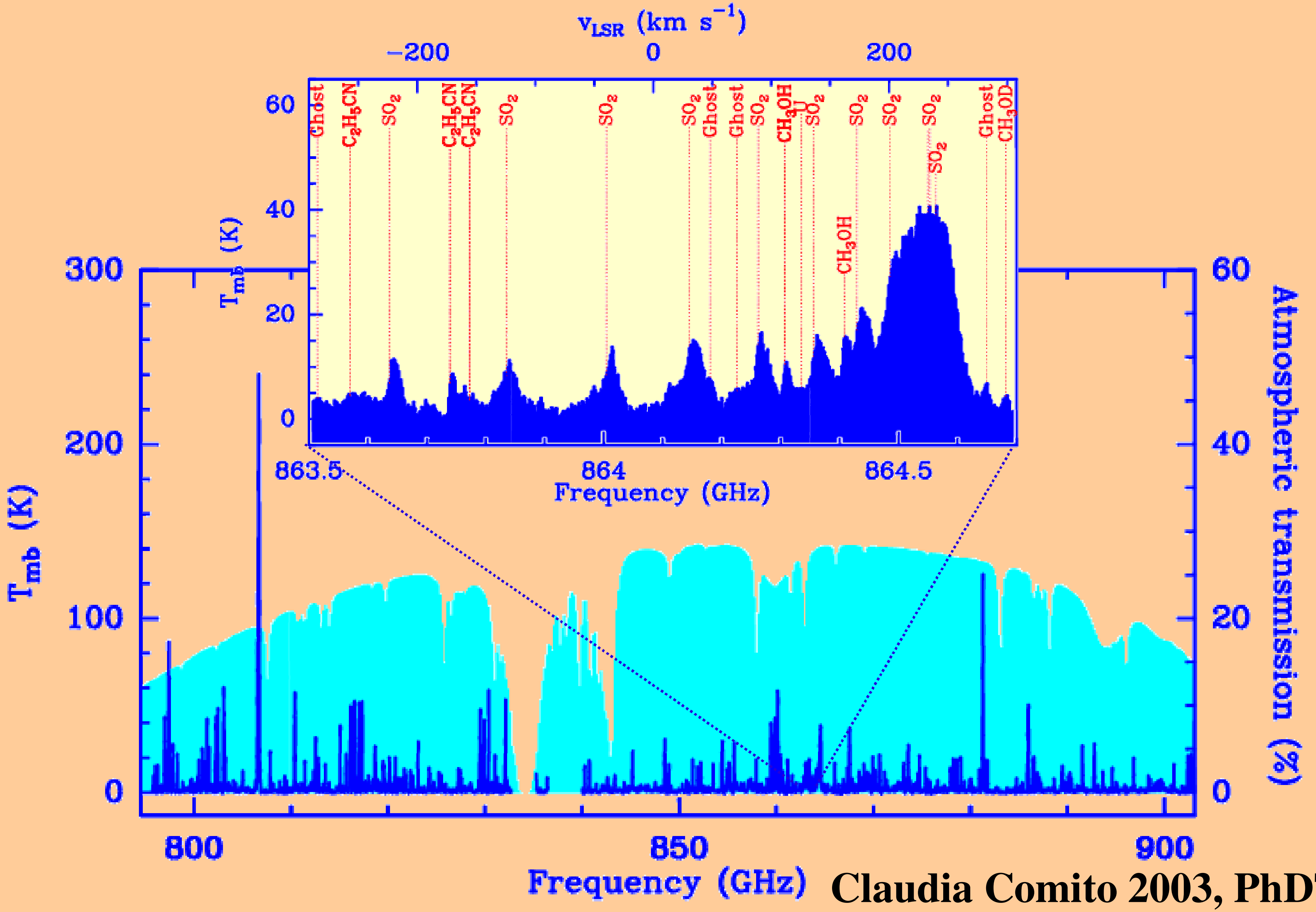
Wright et al., 1996

Claudia Comito 2003, PhDT

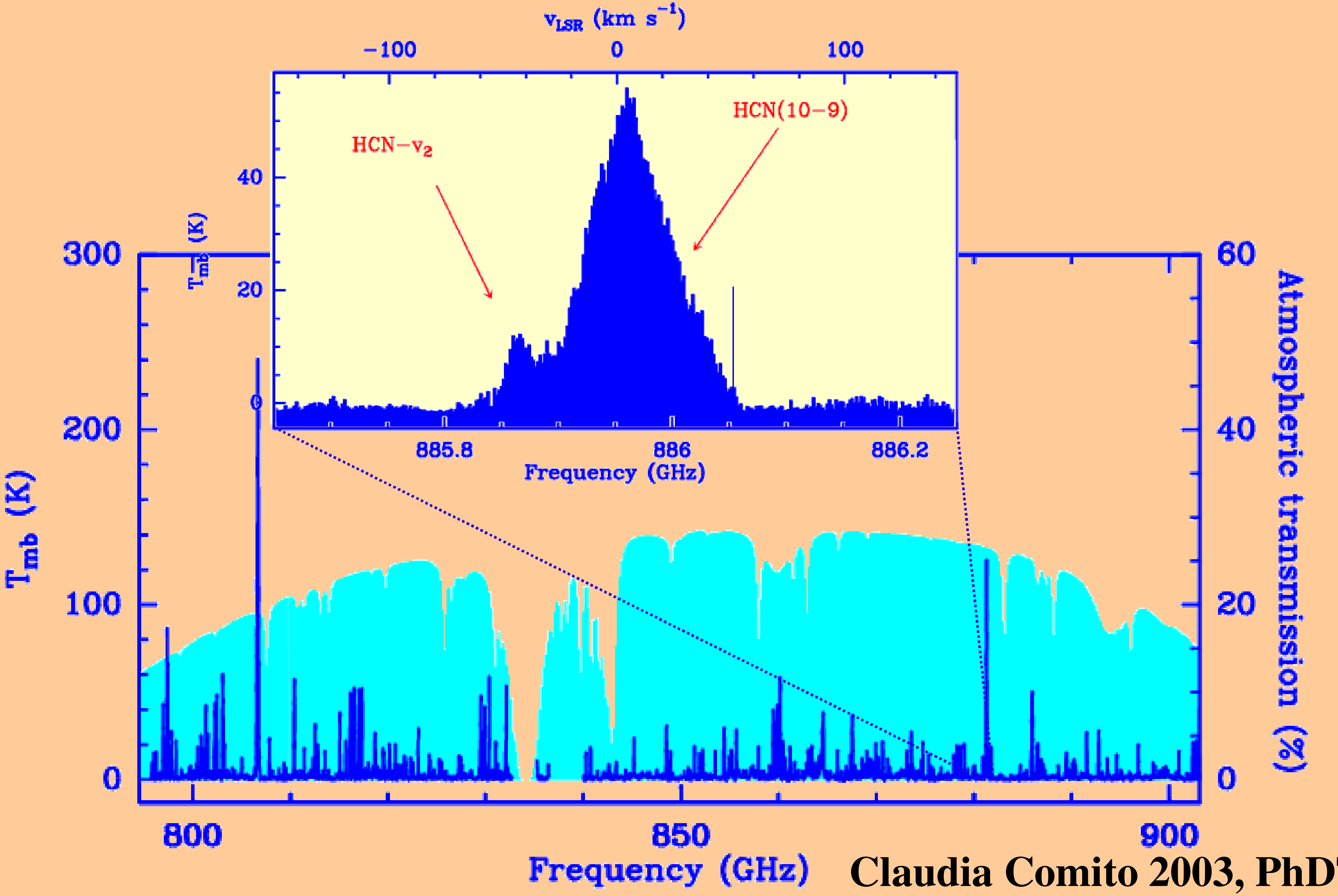
Comito *et al* 2005



Claudia Comito 2003, PhDT



Claudia Comito 2003, PhDT



Claudia Comito 2003, PhDT

ANALYSIS OF THE DATA

✔ *the whole spectrum is fitted at once (Schilke et al. 1997)*

✔*LTE using molecular database (JPL, Cologne)*

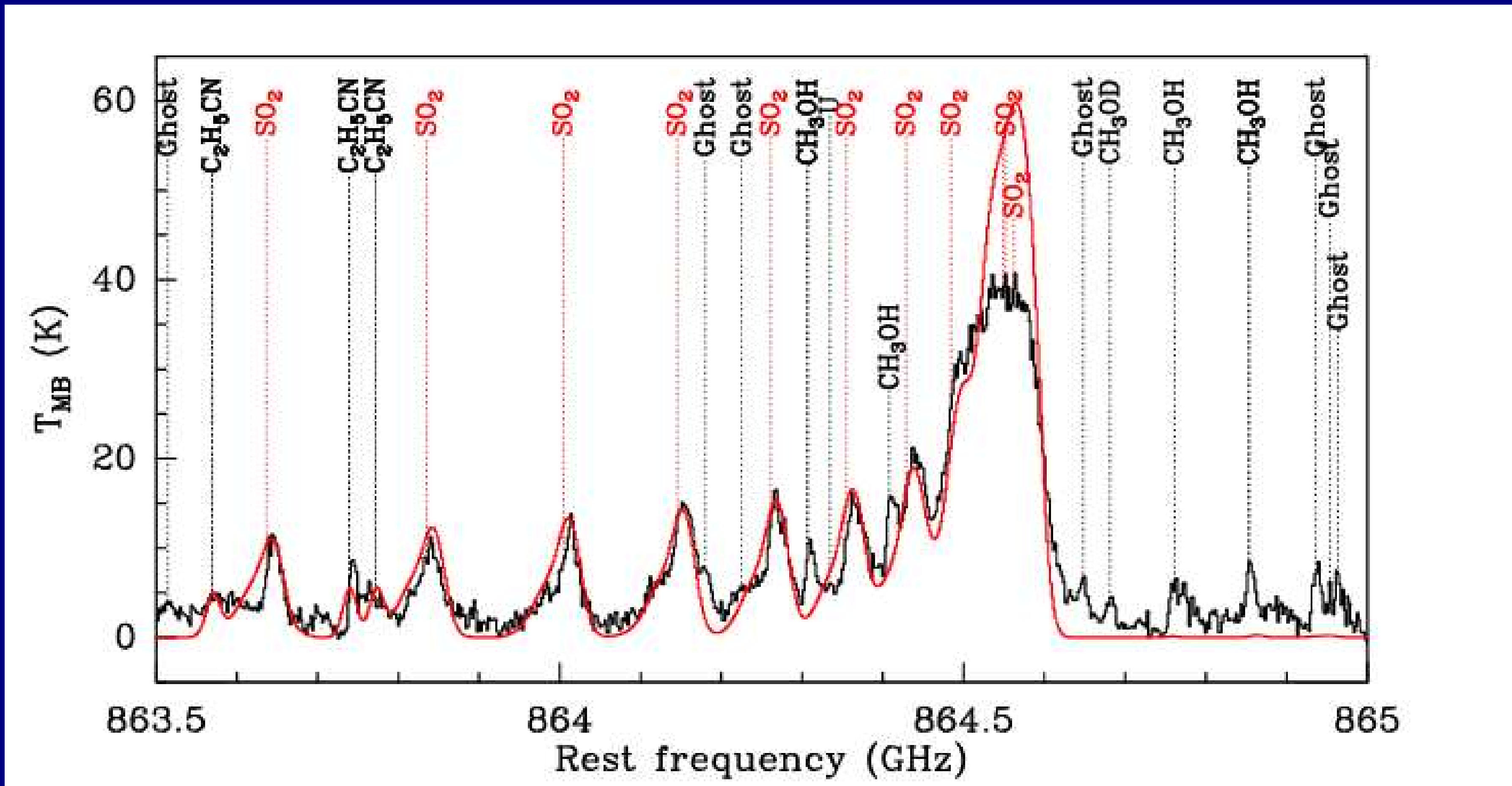
✔ *fits source size, T_{ex}, column density, line width and velocity*

✔ *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!*

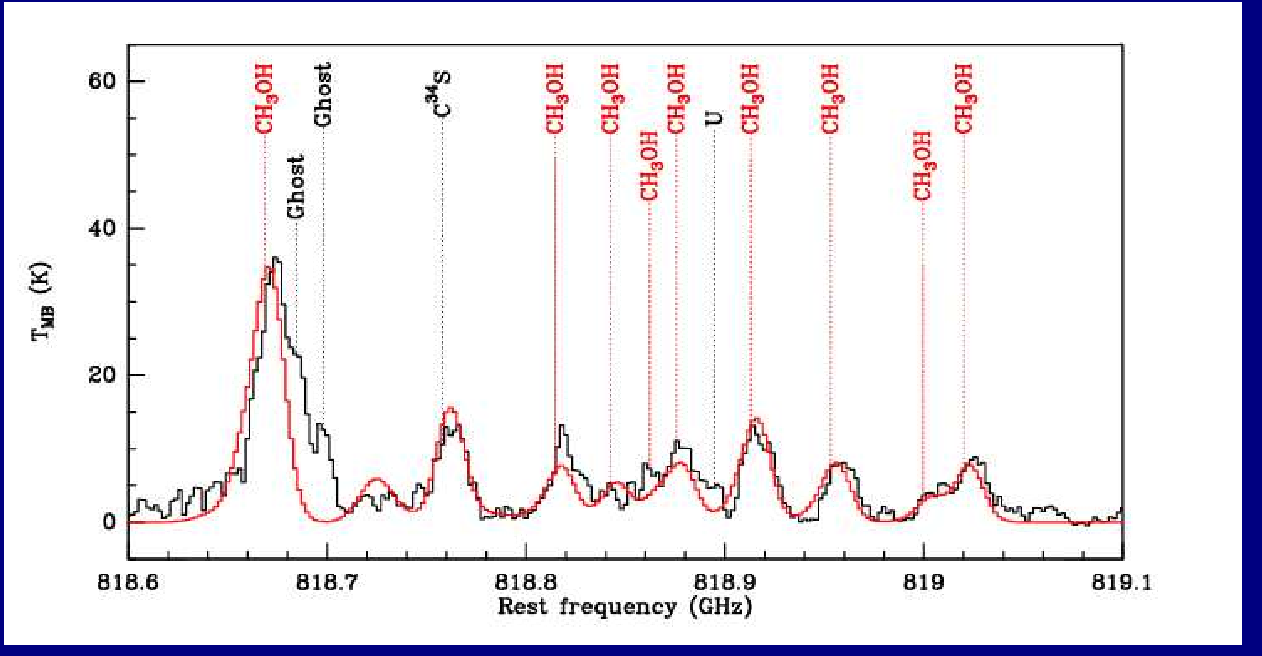
Claudia Comito 2003, PhDT

GOOD FIT: SO_2



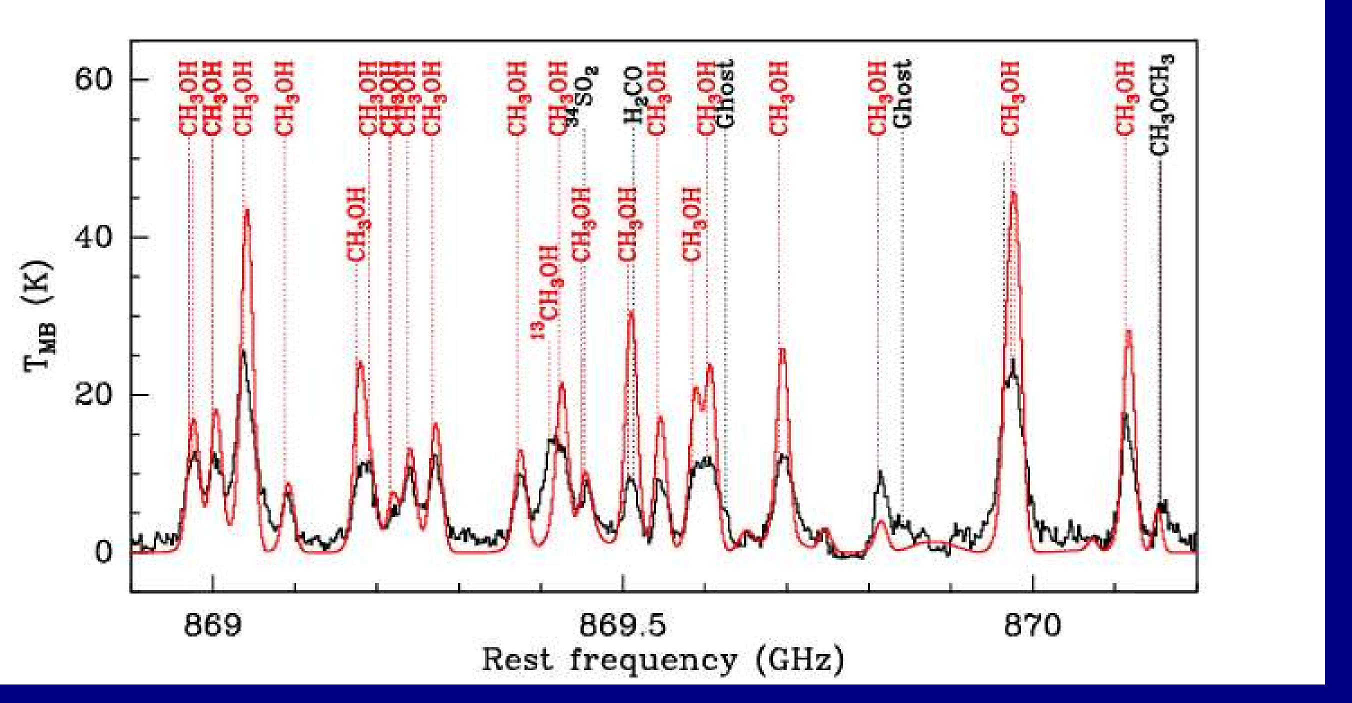
Claudia Comito 2003, PhDT

CH_3OH:



<-- GOOD FIT...

... AND BAD FIT -->



Claudia Comito 2003, PhDT

850-GHz SURVEY: HIGHLIGHTS

With the CSO, we have surveyed the molecular emission of Orion-KL in the 850-GHz band (HPBW=11"). First systematic study in this frequency range!

- ✔ *541 features, 929 transitions from 26 species: even at 350 micron, very rich spectrum! Orion-KL "prototypical hot core"??*
- ✔ *Cooling mostly via SO_2, CH_3OH emission. CO, SO, HCN, H_2CO also contribute significantly.*
- ✔ *Emission from heavy molecules dominating at lower frequencies (e.g., $HCOOCH_3$) disappears. Small hydrides (H_2CO, H_2S, HDO...) kick in!*

Claudia Comito 2003, PhDT

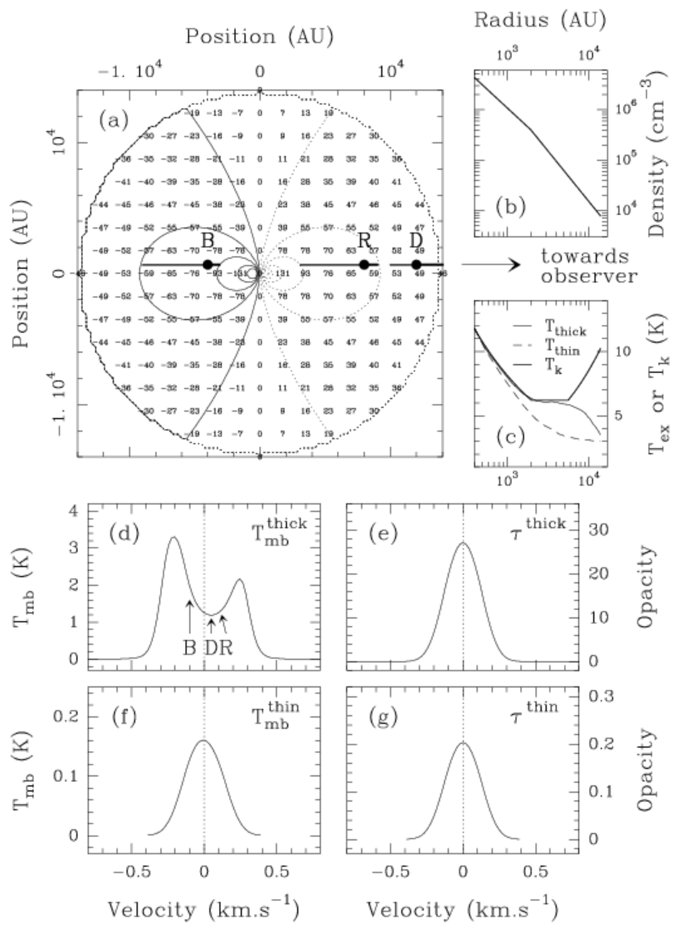
850-GHz SURVEY: HIGHLIGHTS

- ✔ ***Chemical dichotomy Hot Core – Compact Ridge*** ***well represented in the data (complex O-bearing molecules associated with CR, N-bearing species associated with HC).***
- ✔ ***First detections: HNCO (K_a=1-->0) transitions @902 GHz trace the dust radiation field; tentative NH_2 (so far only found in SgrB2), building block of the ammonia chemistry --> FOLLOW-UP OBSERVATIONS!***
- ✔ ***Whole-spectrum LTE analysis carried out for the first time: consistent results, room for improvement (LVG...). Fundamental for future large submm surveys.***

Claudia Comito 2003, PhDT

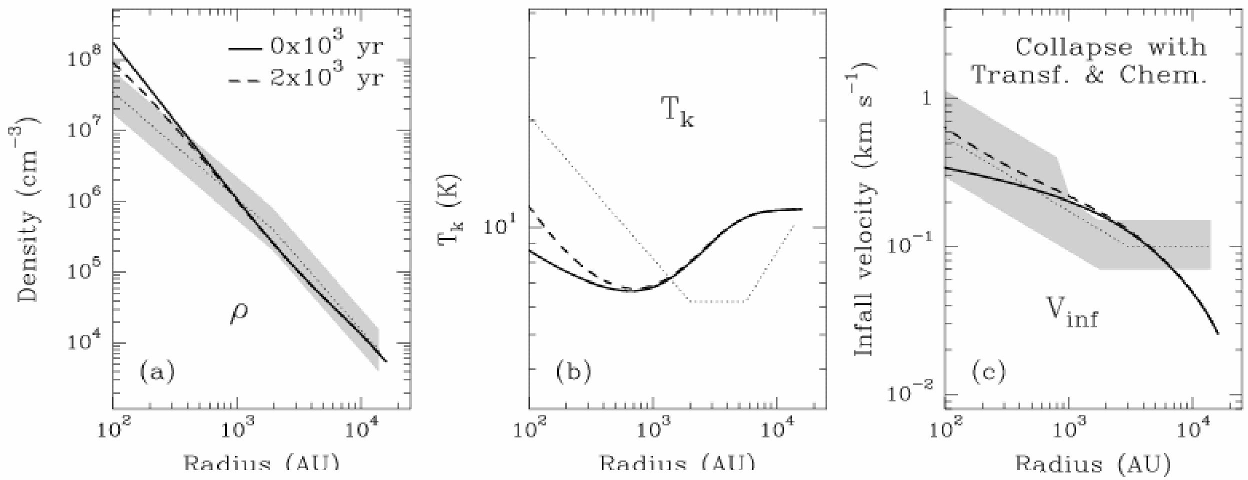
Example II – protostellar collapse

- **Protostellar envelops**
  - Understanding the protostellar collapse
  - The profiles of many lines allow to select the collapse models the closest to reality

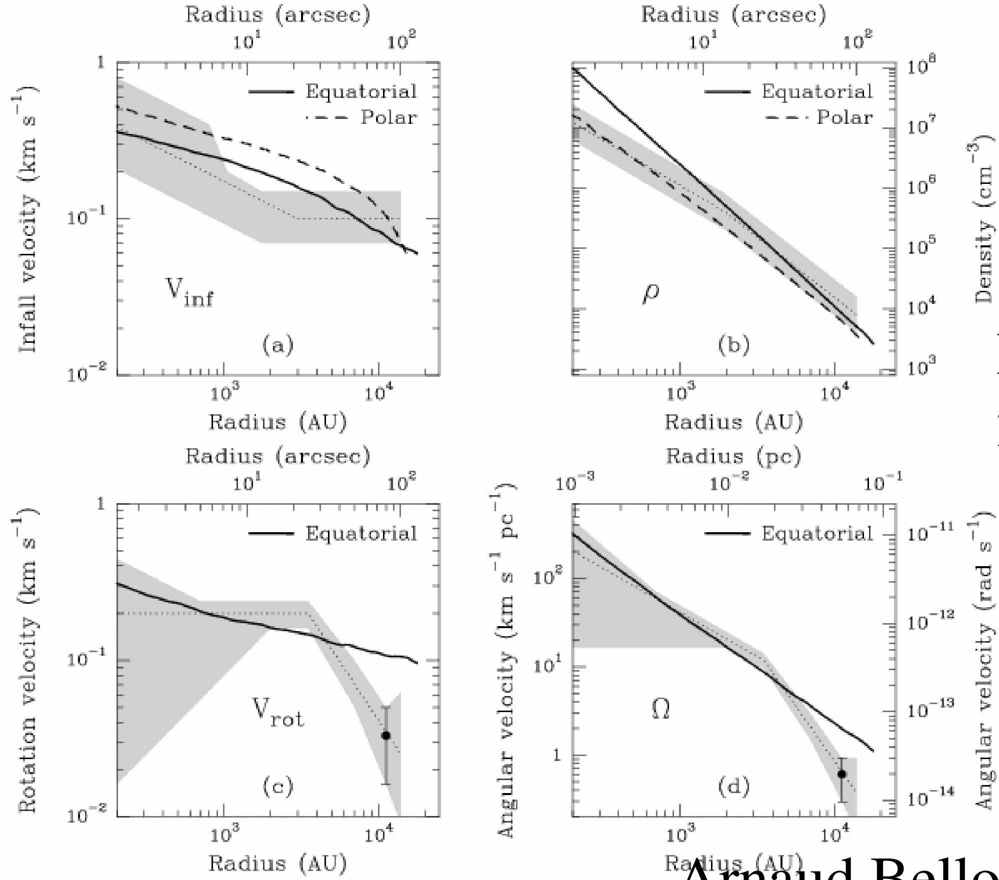


Arnaud Belloche 2002, PhDT

Protostellar collapse models



Lesaffre 2002



Hennebelle 2003, 2004

Arnaud Belloche 2002, PhDT

Example II – protostellar collapse

Collapse model

↓

Radial profiles

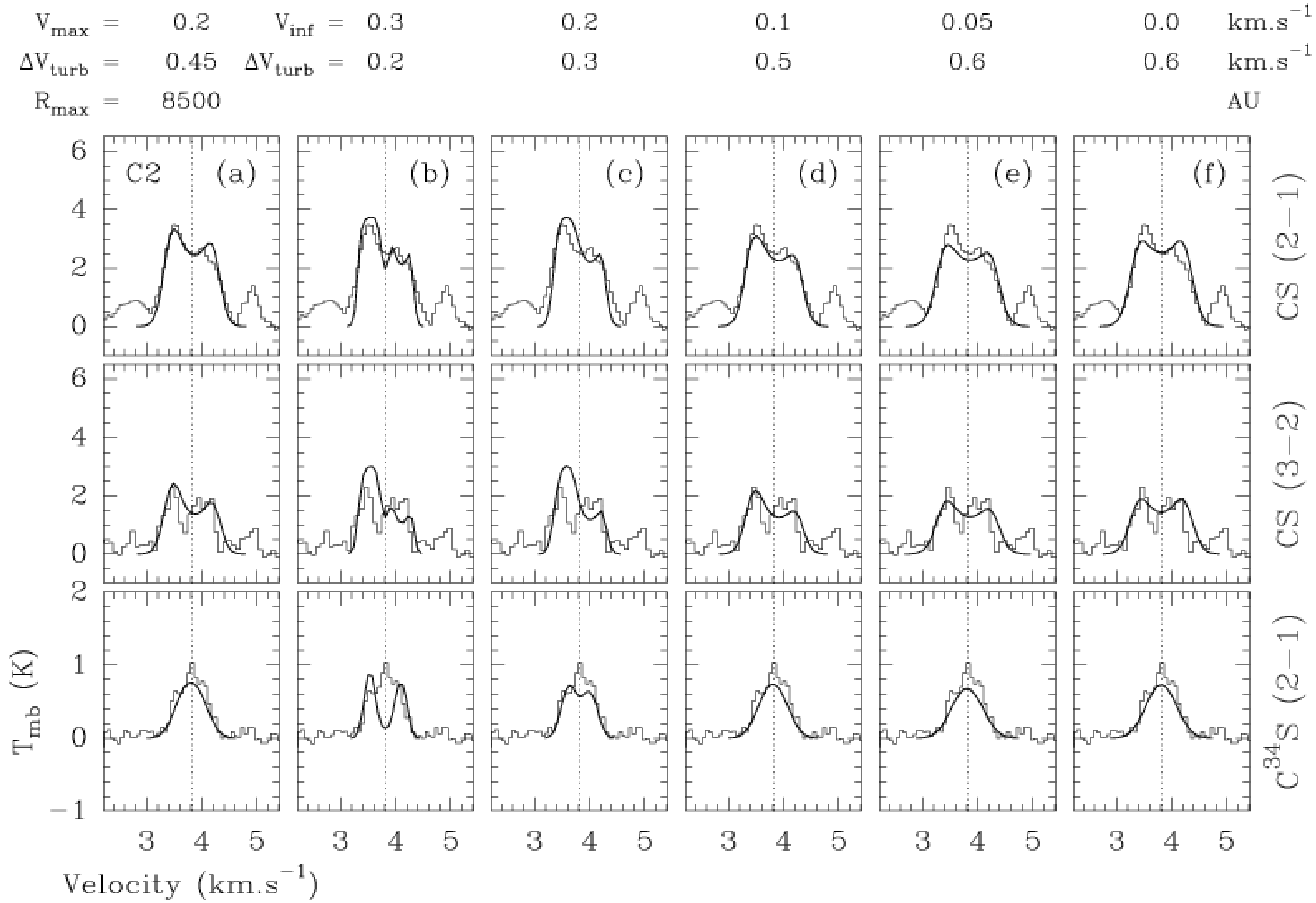
Temperature
Density
velocity

↓

Radiative Transfer
BERNES-MAPYSO

↓

Simulated spectra



Arnaud Belloche 2002, PhDT

Example II – protostellar collapse

Collapse model

↓

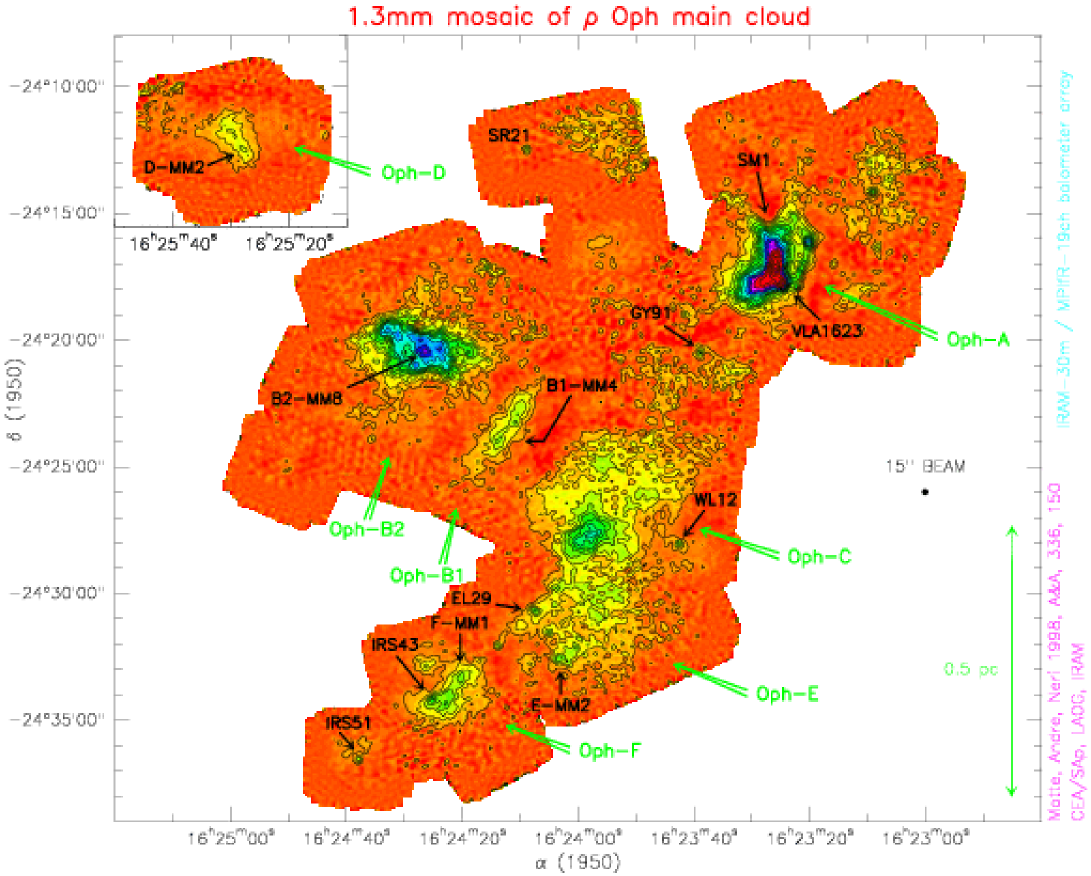
density profile

↓

Radiative Transfert
DUSTY

↓

Simulated continuum map



Arnaud Belloche 2002, PhDT

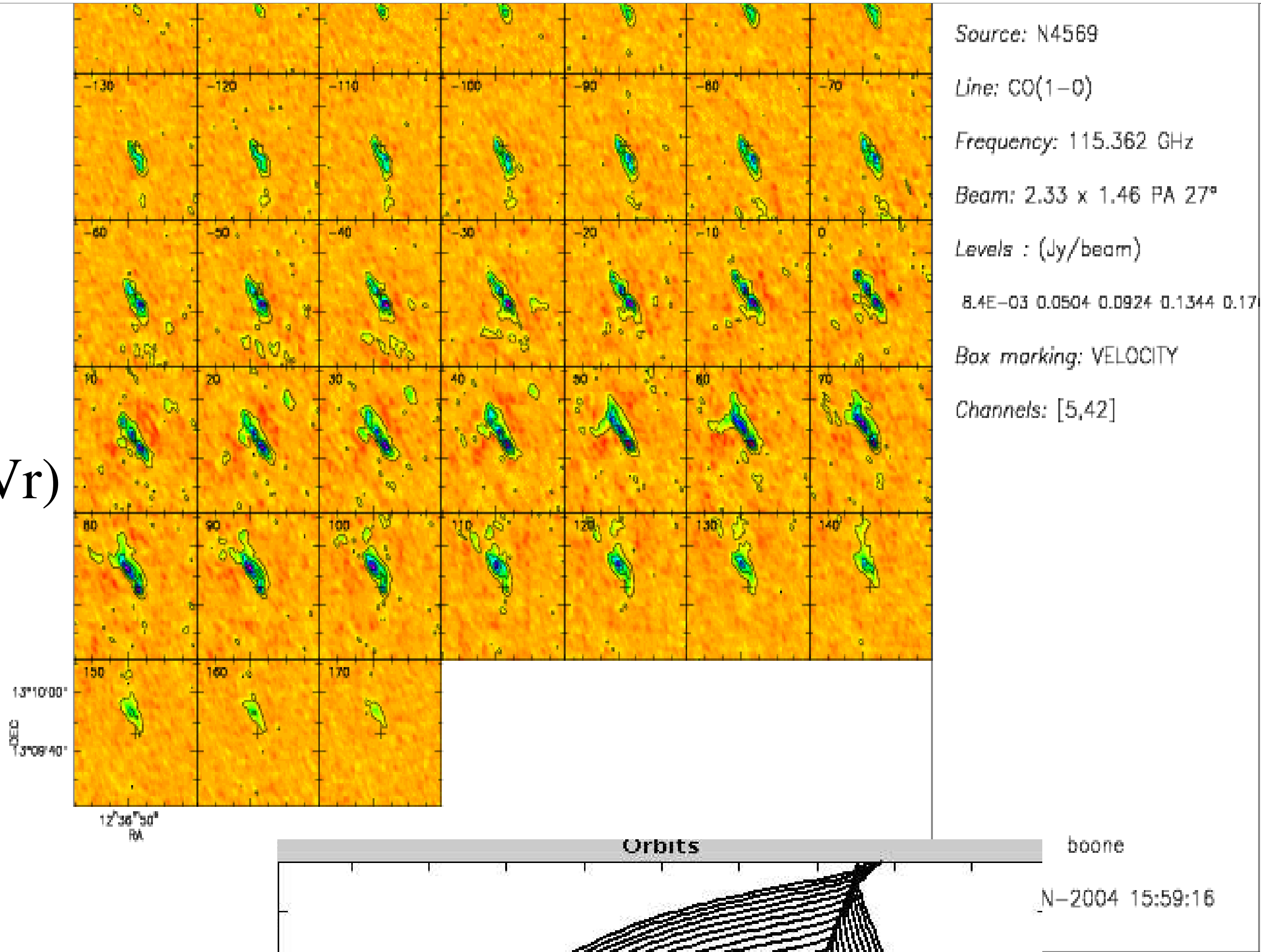
Example III – Galactic dynamics

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

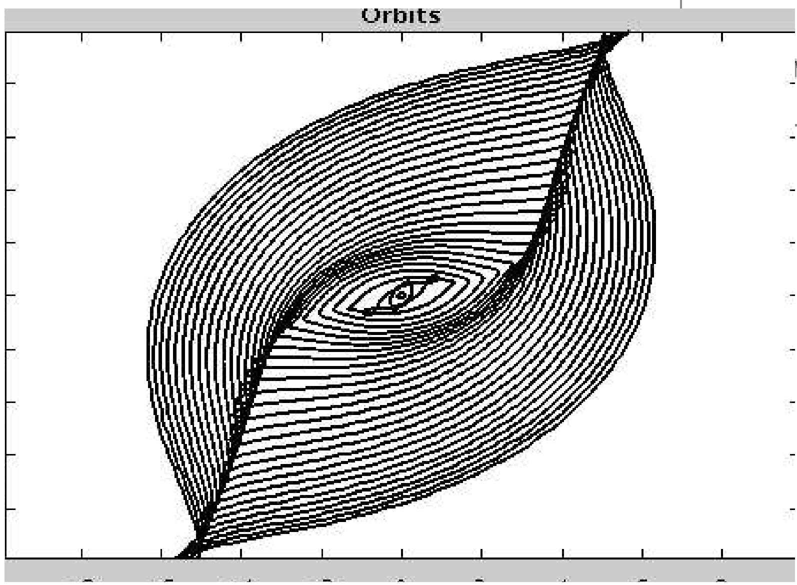
Example III – Galactic dynamics

- **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))



Example III – Galactic dynamics

- **Try several models based on different prescriptions**
  - Tilted rings
  - Bar potential
  - Arbitrary orbital parameters variations

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