Brief introduction to Gildas and MADEX

José Pablo Fonfría

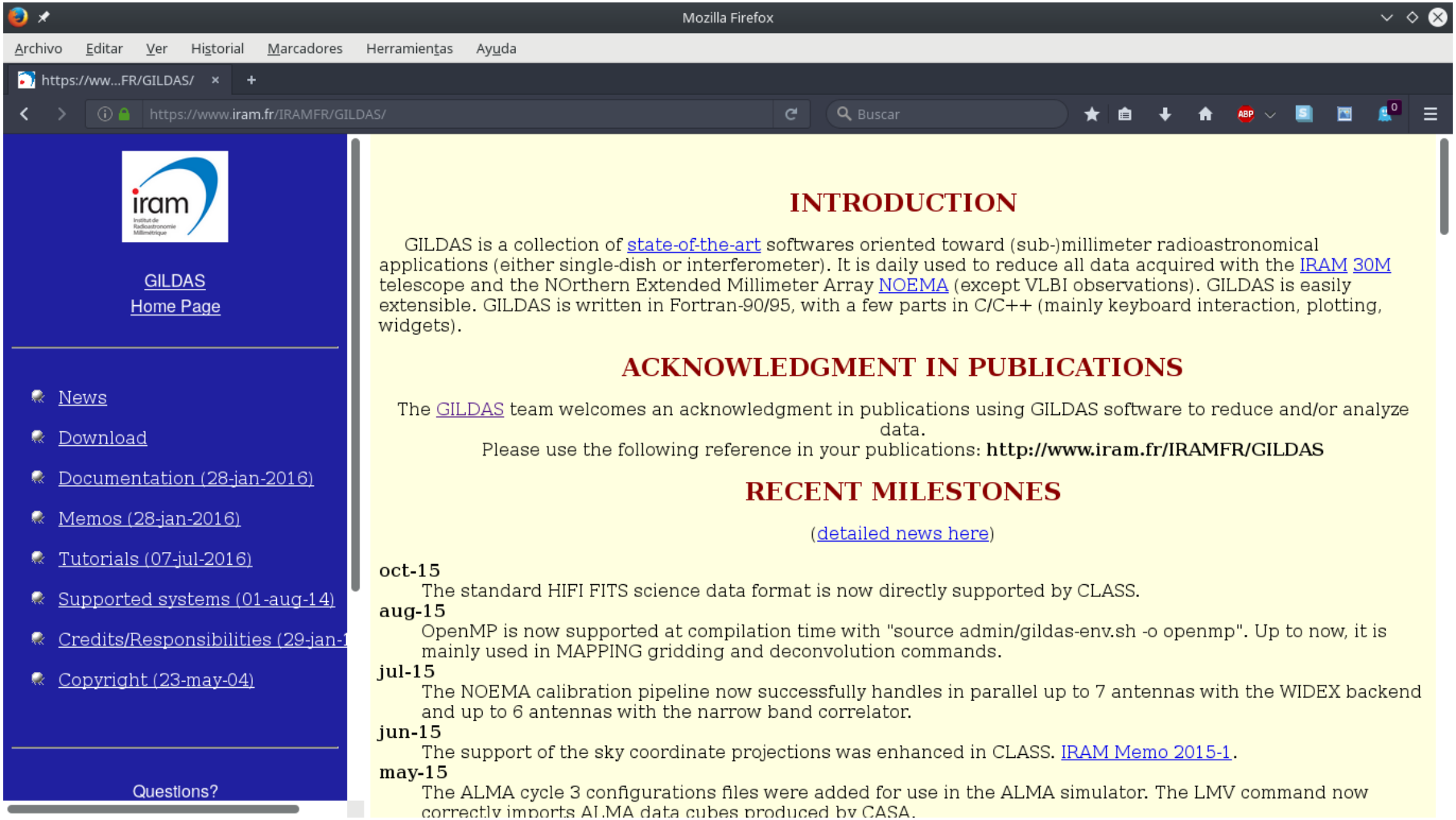
Instituto de Ciencia de Materiales de Madrid (ICMM)
Consejo Superior de Investigaciones Científicas (CSIC)

Guillermo Haro School on Molecular Astrophysics

Instituto Nacional de Astrofísica, Óptica y Electrónica (INAOE)

October 12, 2016

"GILDAS is a collection of state-of-the-art softwares oriented toward (sub-)millimeter radioastronomical applications (either single-dish or interferometer)"



- SIC (*Sympathetic Interpretor of Commands*): It is a command language that can be call by any program as a subroutine.
- GREG (*GREnoble Graphics*): It is used to prepare plots of data or of analysis results. It supports the use of scripts, allowing the user to produce very complex figures.
- CLASS (*Continuum and Line Analysis Single-dish Software*): It is a software package for reducing spectroscopic data acquired with a single-dish telescopes.
- ASTRO (*A Software To pRepare Observations*): This program helps astronomers to prepare observations with the IRAM telescopes.
- CLIC (*Continuum and Line Interferometer Calibration*): This package has been developed to calibrate the data taken with the NOEMA interferometer array.
- MAPPING: Used to deconvolve and map calibrated interferometic data acquired with NOEMA.
- other: TELCAL, MIRA, OFTCAL, MIS

`@<script>.class`: executes a CLASS script with commands inside

`help`: shows a list of all the available commands

- `help <command>`: shows the particular help for the selected command

`file <option>`: opens a data file (*.30m)...

- `file in <file>`: ...to be read
- `file out <file>`: ...for writing purposes (new or old file)
- `file both <file>`: ...to read and write data

`find`: looks for spectra in the opened file fulfilling some conditions. A lot of compoundable options and modifiers can be selected

- `find /all`: looks for all the spectra in the opened file
- `find /frequency` f_1 f_2: looks for spectra with frequencies between f_1 and f_2 (f_1 and f_2 in MHz)
- `find /source <source>`: looks for all the spectra of the source <source>

`list`: shows the spectra found by command `find`

- `list in`: shows the spectra included in the opened file we want to read from (opened with `file in`)
- `list out`: shows the spectra included in the opened file we want to write in (opened with `file out`)

`get <option>`: selects one scan of those found with command `find`

- `get first`: selects the first scan in the list

`get next`: selects the next scan in the list

`get previous`: selects the previous scan in the list

`get last`: selects the last scan in the list

`set <option>`: This command has many options (use command `help set` to see them all)

`set unit <type>`: selects the type of the abscisa axis (C for channels, F for frequency (MHz), V for velocity (km s^{-1}),...). Can provide two types for the lower and upper axes

`set mode <axis> <option>`: selects the scale (<option>) for the chosen axis

`set plot <type>`: selects the way the data are plotted (N: polyline connecting the points, H: histogram, P: points)

`modify <option>`: edits the entries of the observation header

`modify frequency <value>`: changes the central frequency (used to calculate the Doppler velocity)

`stitch`: makes the union of all the spectra found with `find`

`stitch /nocheck`: useful to deal with old observations

`average`: averages all the spectra found with command `find`

`plot`: plots the observed data and the observation header

`draw <option>`: gives information of the selected channel if no <option> is provided. It can be used to flag or interpolate bad channels or write text on the spectrum box, among others.

`hardcopy`: creates a hardcopy of the current plot usually in EPS format

BASELINE REMOVAL

`set window`: defines windows to avoid during the fitting process

`base <degree>`: fits the baseline of an spectrum with a polynomial of degree <degree> and substracts this polynomial from the spectrum (copies buffer R to T before performing the fit)

`swap`: exchanges the content of the R and T buffers

LINE FITTING

`method <method>`: selects the method to be applied during the fit to the observed line. There are four method: GAUSS, SHELL, NH3 and HFS. The last two method are useful to deal with lines with hyperfine structure

`lines <n> <guesses>`: selects the number of lines <n> to be fitted at the same time. If <n> is higher than 0, it is necessary to provide estimates of some parameters. If <n> is 0, `minimize` tries to guess these parameters.

`minimize`: fits the lines selected with command `lines`

`iterate`: if `minimize` does not converge, thist command is used to improve the fits

`visualize`: shows the fit to the <n>-th line selected with command `lines`

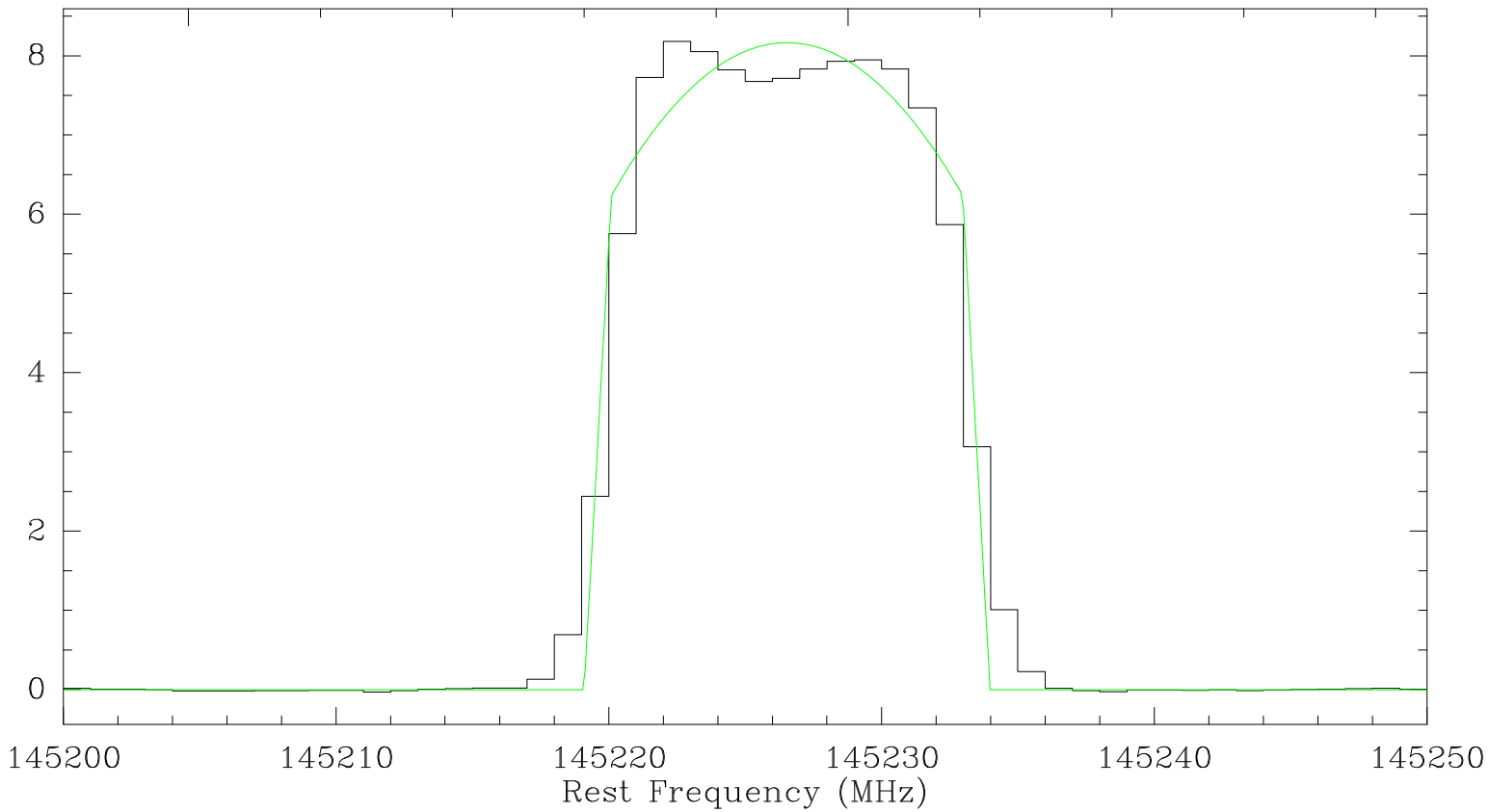
`residual`: calculates the residuals of the last fit of the <n>-th line selected with `lines`

A SIMPLE EXAMPLE

Looking for line SiS(8 – 7) at ≃ 145 GHz in 2mm_survey.30m

```
1: file in 2mm_survey.30m
2: find /frequency 145200 145300
3: stitch /nocheck
4: set mode x 145200 145250
5: plot
6: set window (interactive)
7: base 0
8: modify frequency 145227.0530
9: method shell
10: lines 1 0 104 0 -1 0 13 0 1.2
    (interactive)
11: minimize
12: visualize
13: hardcopy example_sis8-7.eps
```

0;0 IRC+10216 Unknown IRAM−30M−B30 0:13−MAR−1987 R:08−OCT−2016
RA: 09:45:14.80 DEC: 13:30:40.0 Eq 1950.0 Rad. 0.0° Offs: +0.0 +0.0
Unknown tau: 0.098 Tsys: 739. Time: 7.26E+02min El: 50.7
N: 1953 I0: 696.500 V0: −27.00 Dv: −2.068 Unkn
F0: 145000.000 Df: 1.000 Fi: 153718.756



`@<script>.greg`: executes a GREG script with commands inside

`help`: shows a list of all the available commands

`help <command>`: shows the particular help for the selected command

`set plot_page <option>`: select the canvas geometry. The option can be `landscape`, `portrait`, or the width and height can be provided

`column x 1 y 2 /file <file>.dat` : opens a reads the first and second columns of file <file>.dat assigning the first column to the abscisa axis and the second one to the ordinate axis

`limits`: calculate the limits of the read data to plot the whole set

`limits` $x_{\min}$ $x_{\max}$ $y_{\min}$ $y_{\max}$: provide GREG with the desired limits. Any number can be changed by $=$ or $*$ to keep the previous number or to let GREG to choose the highest/lowest value

`limits /xlog`: the x-axis is expressed in logarithmic scale. /ylog can be used for the y-axis. Both modifiers can be used at the same time

`box`: plots a box with the current limits

`axis <name>`: plots an axis (`xlow`, `xup`, `yleft`, `yright`). This command accepts several modifiers

`connect`: connects the points defined by vectors x and y read with command `column` with straight lines.
- `connect` a b: connects the points defined by vectors a and b

`curve`: builts the cubic spline interpolation for vectors x and y

`histogram`: plots an histogram for vectors x and y

`points`: plots isolated points for vectors x and y

`draw`: gets the coordinates of a selecte point in the canvas
- `draw relocate`: chooses an initial point
- `draw line`: draws a straight line from the initial point to a new point
- `draw arrow`: draws an arrow from the initial point to a new point
- `draw text`: puts a character string in the selected point

`set`: controls many GREG parameters

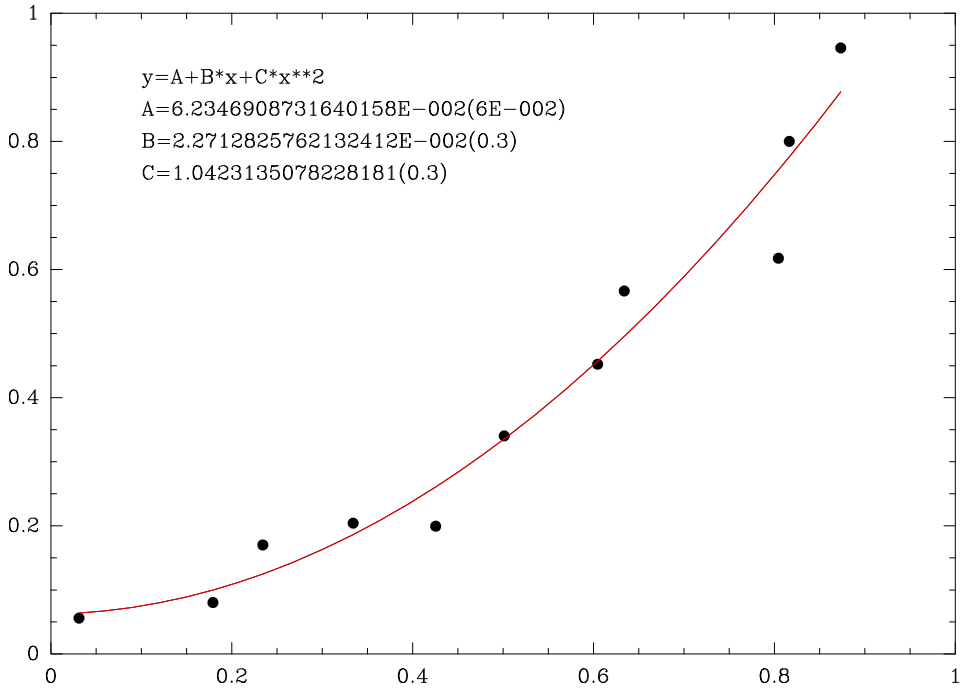
FIT TO A DATA SET

`mfit <function>`: performs least squares fit to a data set using the function <function> defined by the author. The syntaxis is `mfit` $y =$ `f`$(x; \&A, \&B, ...)$

`connect x mfit %fit`: plots the fitted function

A SIMPLE EXAMPLE
Fitting a data set

```
1: column x 1 y 2 /file data.dat
2: limits
3: box
4: set marker 12 3 .3
5: points
6: mfit y=&A+&B*x+&C*x**2
7: pencil /c 1
8: curve x mfit %fit
9: draw text 0.1 0.9
"y=A+B*x+C*x**2"6 0
10: draw text 0.1 0.85
"A=6.2346908731640158E-002(6E-002)"6
11:draw text 0.1 0.8
"B=2.2712825762132412E-002(0.3)"6 0
12:draw text 0.1 0.75
"C=1.0423135078228181(0.3)"6 0
13: hardcopy mfit_fit.eps
```



- MADEX (MAdrid EXcitation code) is a powerful program developed by J. Cernicharo (Cernicharo, 2012, EASP, 58, 251) over the last 30 years that takes advantage of the Sobolev approximation to calculate the pure rotational spectra of a large number of molecules, some of them unavailable in the well-known CDMS or the JPL catalogs.
- It uses the newest spectroscopic and colisional data available, which allows the user to model a large number of molecules that other codes cannot deal with.

Comparison between the frequencies of some lines available in the MADEX code and the results found in other public databases (CDMS, JPL).

Molecule	Transition	MADEX	Database	Reference
CO	J=5-4	576267.9311(2)	576267.9305(50)	CDMS
CO	J=20-19	2299569.8627(25)	2299569.842(10)	CDMS
CO	J=40-39	4564005.784(30)	4564005.640(53)	CDMS
CO	J=50-49	5672166.88(23)	5672165.67(55)	CDMS
HCO^+	J=4-3	356734.2246(11)	356734.2230(15)	CDMS
HCO^+	J=23-22	2047315.5(11)	2047315.0(10)	CDMS
CS	J=10-9	489750.9216(10)	489750.9210(38)	CDMS
CS	J=40-39	1949392.438(84)	1949392.410(78)	CDMS
CCS	$N_J=17_{16}-16_{15}$	219142.6745(67)	219142.6745(85)	CDMS
CCO	$N_J=7_6-6_5$	161729.4443(35)	161729.4330(80)	JPL
CCO	$N_J=22_{21}-21_{20}$	507782.82(28)	507782.80(22)	JPL
CH_3CH_2CN	$JK_aK_c=32_{2,30}-33_{1,33}$	44894.583(15)	44894.588(11)	JPL
CH_3CH_2CN	$JK_aK_c=12_{3,10}-13_{1,13}$	94015.876(5)	94015.901(4)	JPL
CH_3CH_2CN	$JK_aK_c=37_{4,33}-38_{1,38}$	322400.259(24)	322400.329(17)	JPL
TiO	J= 5-4 Ω=2	160108.271(11)	160108.244(22)	CDMS
TiO	J=10-9 Ω=1	316518.993(9)	316518.994(40)	CDMS
NiO	$N_J=19_{19}-18_{18}$	575661.654(22)	575661.656(94)	CDMS
HC_5N	J=50-49 ν_{11} e	133337.7989(26)	133337.8009(35)	CDMS
HC_5N	J=50-49 ν_{11} f	133453.5559(22)	133453.5596(25)	CDMS

`@<script>.mlvg`: executes a MADEX script with commands inside
`help`: list all the available commands
  `help <command>`: shows a brief help about the selected command
`defa`: shows the current parameters considered by the program
`find <modifier>`: looks for specific molecules/atoms in the list
  `find /mole`: looks for molecules in the list
  `find /atom`: looks for atoms in the list
`list <n>`: list the molecules with n atoms
`mole`: selects the molecule to analyze
`nrot`: selects the number of considered rotational levels
`nvib`: selects the number of considered vibrational levels
`tk`: selects the kinetic temperature
`tvib`: selects the vibrational temperature
`tetl`: selects the rotational temperature
`spec`: shows the spectroscopic information about the selected molecule
`wrot`: writes on screen the spectroscopic constants of the selected molecule
`ener`: writes on screen the energy of the molecular levels
`cd`: provides the column density of the selected molecule
`a13c, a17o, 37cl, 29si,...`: ask for different isotopic ratios

`rad`: introduces the radius of the cloud
`geom`: changes the geometry (spherical, plane-parallel)
`vexp`: selects the gas expansion velocity
`vlsr`: selects the systemic velocity of the source
`dist`: distance to the source
`lte`: computes LTE populations, opactities and brightness temperatures for the selected molecule
`mlte`: computes LTE populations, opactities and brightness temperatures for the selected molecule and all of its isotopologues
`exec`: solves the statistical equilibrium equations and writes the brightness temperature on screen for the selected molecule
`mexe`: solves the statistical equilibrium equations and writes the brightness temperature on screen for the selected molecule and all of its isotopologues
`wspe`: writes the calculated spectrum to a file
`fre1/fre2`: provides the lower and upper frequencies of the spectral range considered by command `wspe`