The Gifa Basic Documentation

THE GIFA PROGRAM.

This program has been developed in several NMR groups in France, first in I.C.S.N. in Gif/Yvette, then in Ecole Polytechnique in Palaiseau and now in Montpellier under the coordination of Marc-Andre Delsuc. Please contact :

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This program can be downloaded by anonymous FTP on Internet, the home site is the following address : ftp://www.cbs.univ-montp1.fr/pub/gifa_v4. The home page of Gifa on WEB is : http://www.cbs.univ-montp1.fr/GIFA/welcome.html.

PRESENTATION

The Gifa program is a multi-purpose NMR program. It is designed for the processing, the display and the analysis of 1D, 2D & 3D NMR data-sets.
The program includes all the classical processing, displaying and plotting capabilities of an NMR program, as well as more advanced processing techniques and assignment facilities. There is no actual limit to the size of the data-set which can be processed. A complete macro language permits to builds sophisticated processing. The Graphic User Interface is fully designable and programmable by the user.
The program currently runs on several UNIX platforms. The graphics can be displayed on X-Windows terminals. Plots are generated on postscript or HP-GL devices.
The version 4.4 is a stabilized version, however it is evolving all the time, check our ftp server ! This version is distributed under a licence, the licence requires that you refer to Gifa in any published work which depend in some manner on the Gifa program.
This program can be downloaded by anonymous FTP on Internet, the home site is at the following address : ftp://www.cbs.univ-montp1.fr/pub/gifa_v4 .

Classical processing includes :

- Full capabilities in 1D, 2D and 3D processing.
- Full array of apodisation functions (shifted sine-bells and squared sine-bells; exponential; Gaussian; trapezoid, and combinations) - Zero-filling and truncation.
- Fast Fourier transform (direct and inverse; real, complex, and hypercomplex). Hilbert transforms.
- Phasing of 1D, 2D and 3D spectra.
- Processing in memory (for regular data size) or on disk (for very large data-set) with similar syntaxes.
- Non-limited size data-set with optimised file access protocol.
- Very fast processing : recently test on a PIII 800 MHz

the complete processing of a 512x2048 data points data-set, including :
windowing in F2, shifted sine bell in F1.
FT with zero-filling in F1 and phasing in both axes.
spline baseline correction through 5 points in F2.

- Post-processing filters; modulus, real part extraction, absolute value, smoothing, etc...
- Complete baseline correction module (linear, cubic spline correction, and a comprehensive polynomial module with automatic peak detection).
- Extraction of sub-spectra for local processing.
- Simulation of pseudo data-sets. Simulation of 2D NOESY from intensity files (CORMA type)
- Symetrisation, projections

Graphic capabilities :

- 2D Displays in -density mode -contour mode -stacked plot mode.
- 3D Display in 3D perspective.
- Random access to rows, columns, diagonals or projections in 2D mode.
- Random access to planes and rows in any direction or diagonals in 3D mode.
- 2D strip files and strip plots from 3D.
- Multi-windowing facilities : up to 4 active windows in the same time, many passive windows.
- Correlated cursors between windows.
- Fast zoom mode - Fast interactive phasing mode.
- Possibility to superimpose on screen several 1D or 2D spectra.
- Complete plotting facilities. On screen : 1D plots; 2D : full colours density maps, zoom, contour plots and stacked plots; 3D : automatic series of 2D plots, 3D graphics. All 1D, 2D and 3D graphics may be sent to a plotter (HP-plotter or PostScript laser printer). Several plots may be disposed on the same sheet of paper, and plot files can be stored separately.

Special processing includes :

- A protein assignment module is available for 2D homonuclear spectra. Completely written in the macro language.
- Maximum Entropy processing of 1D as well as 2D data-sets. A generalized iteration scheme, (Gifa stands for Generalised Iterative Fixed-point Algorithm) as well as more classical algorithms : Gull & Daniel, conjugated gradients.
- Maximum Entropy deconvolution of Lorentzian line-shape, of J-coupling pattern, or of any user-provided function.
- Comprehensive Linear Prediction module, including Burg, LP-SVD, forward and backward methods, etc
- Processing of DOSY experiments, using either Maximum Entropy for complicate (polydisperse) analysis, or a simple fitting technique.
- Automatic peak-picker in 1D 2D and 3D; Automatic peak integrator in 1D and 2D.
- Line fitting of mixed Lorentzian and Gaussian Line Shapes.
- A generic fitter which permit to fit arbitrary functions to the data-set.
- Several file formats are available, notably a MATLAB compatible format, a compressed format, a generic file format, permitting direct random access, and several others.
- A Protein assignment module and complete relaxation analysis of HSQC. A NMRstar compatible format, a XPLOR/CNS output format.

A Complete set of Macro :

- A complete graphic user interface written in the macro language.
- Simplified user interface for 2D processing and plotting, permitting a fast access to the program.
- Calibration, integration, peak-picking, etc..
- Fast interaction with the mouse on 1D, 2D and 3D.
- Easily extensible with the control language.

The User Interface is characterized by :

- Most command are available through a flexible graphic interface.
- Interactive commands for beginners as well as fast entry mode for advanced users.
- Complete on-line HELP.
- Comprehensive on-line manual.
- Versatile command parser which permits to build macro commands with alias, tests, local and global variables, loops, graphic interaction and display capabilities, support for data-bases and associative arrays.
- Graphical interface completely modifiable and definable by the user.
- Possibility to run in interactive mode as well as Batch mode (display less).
- Command line history and command line editing.
- The operating system is fully available from Gifa.

FIRST CONTACT WITH THE PROGRAM.

Entering the program

First insure that the program have been correctly installed from the distribution kit, contact your system manager or your local expert.
You enter the program by typing `gifa` on your favourite system. The program should give you a short greeting, the size of the larger data-set, and then respond in the text window with the prompt :

```
Gifa>
```

If every thing as been set up correctly, you should also see two spectral windows, a horizontal menu bar and a control box showing off. To get the graphics, you should make sure that the environment variable DISPLAY has been correctly set to point on your current terminal (with the command setenv DISPLAY when running UNIX). If no X display is available, Gifa will tell you that no graphic will be available, but will start correctly however.
If you experience problems when starting Gifa, check the FAQ at the end of this manual.

Principe of operation

There are two ways of issuing commands to Gifa. The first one is to type commands directly in the text window, at the prompt level. Such commands are of two kinds, built-in commands, directly executed by Gifa, and macros, which are command files written in the Gifa command language. From the user level, there is little difference between the two kind of commands.
The other method consists in clicking on a button in the graphic interface. The graphic interface is mostly composed of two types of objects: a menu bar, holding sets of related commands; and forms which may reside on screen, and can have additional parameters.
The two methods are strictly equivalent, graphic buttons are internally associated to commands (or list of commands). One day, you will eventually learn how to do your own buttons.
Graphic windows can be closed at any time, simply by clicking on their close-box. The 1D window, the 2D contour-plot an the 3D cube window can also be resized. However in certain cases (resizing a 1D in 2D mode for instance, or when a complex drawing has been set, or with the 3D display), the image in the window can be lost for a short time. **However the data can never be damaged in any manner.**

Entering Parameters

You are now ready to enter your first command. If you hit the `About GIFA` button in the **`File`** menu, you will get a short introduction.
Entering

```
Gifa> help
```

at the prompt level will give you the same message. With this version of Gifa, help is actually a macro. Their are also built-in commands. Macros are case sensitive (you call them by their file-name) but built-in commands are not. In the whole manual, we will use the rule that every built-in Gifa command is given in uppercase. Macros, however have to be typed exactly as defined (this is due to the UNIX file-system), they will always appear in the manual as lower case.
Typing

```
Gifa> hulp
```

will give you an error message, since there is no command nor macro named hulp (at least on the distribution kit)!
help can also be used with a parameter :

```
Gifa> help primer
```

Some command may require one or several parameters, you will be prompted for such parameters, either in graphic dialogue boxes if the command was entered from a menu, or at the text terminal if the command was typed from it. When entering the prompt level, it is also possible to put the parameter directly after the command on the same line.
For instance, let us try the *UNIT* (built-in) command which permits to determine the current unit used on the data-set : PPM, Hertz (as determined form internal parameters), Index (ranging from 1 to n in the case of a data-set of length n), seconds (for time domain data-sets), damping (for DOSY experiment) or tabulated (for arbitrary, user defined units).
Typing

```
Gifa> UNIT
```

will prompt you for the unit to use, just typing return will leave the value unchanged.
Typing

```
Gifa> UNIT H
```

Will set the current unit to Hertz.
On the other hand, clicking on the Unit button, in the **Move** menu will pop-up a dialogue box which

realises the same thing.

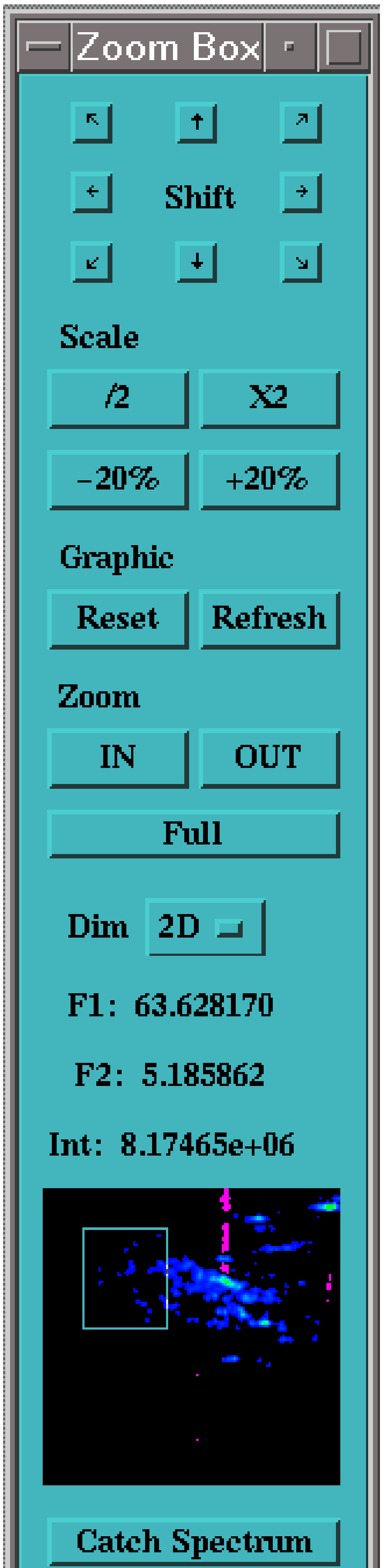
BASIC GRAPHIC USER INTERFACE

The standard graphic interface is characterized by several graphic windows and controls used for the display of the spectral data, and by a set of menus, button boxes, and dialogue boxes used for graphic user interaction.

Display

Several graphic windows can be opened at the same time within Gifa. By default, when entering the program, a 1D display and a 2D density display window are opened. Several other graphic windows can also be opened (see for instance CDISP2D, DISP3D, FREEZE). The data held in the working buffers are shown in these windows.
These windows can be closed at any time, re-opening them is performed by issuing the correct command either from the prompt or from the menus (see below). Most of these windows can be resized, to the exception of the 2D density display window which has a fixed size of 512 pixels on each axis. The colors in these windows can also be modified with a set of colour commands.
All the spectral windows can be FREEZE, either by typing the command, or by selecting the entry in the window menu. A frozen window is just a copy of the current window, just staying here for comparison. It is completely passive, and can only be closed or iconified if needed, the content cannot be changed anymore.
The graphic windows are completely optional, and the effect of a command does not depend on the fact that a graphic window is there or not to display the effect.

Zooming



A control box (Shown here) should also appear at start-up in the upper right corner of the screen. This box holds controls which permits to zoom and adjust the scale of the display. (If this box disappears, or is absent for any reason, you can make it appear again with the `ZM` command (also in the **Display** menu)).
There are many ways for selecting a zoom window in Gifa. Apart from the direct command `ZOOM` (see this command), you can simply click on the graphic window with the left and middle buttons pressed at the same time (or Shift+left button), and draw a rectangle on the display. You can redraw as many time as wished this rectangle. Zoom into the selected region, simply by clicking in the window with the left and right button of the mouse (or Shift+right button). You can also use the Zoom in and Zoom out buttons in the control box. Of course the Full button resets to the full spectral view.
Here is a summary of the possible actions.

Action	Mouse Buttons	Shift + Buttons
Draw Selection	left + middle	left
Zoom in	left+right	right
Zoom out	middle+right	middle

The control box holds a miniature spectrum of your 2D data-set, it was displayed when you clicked on the Catch Spectrum button. The white rectangle in it, shows the current zoom region. You can also move around the little zoom box in this window with your mouse, and the zoom will move accordingly.
The 8 little arrows on the top of the zoom box can be used to move around the zoom region. Each arrow will move the selected region by half the size of the zoom box.

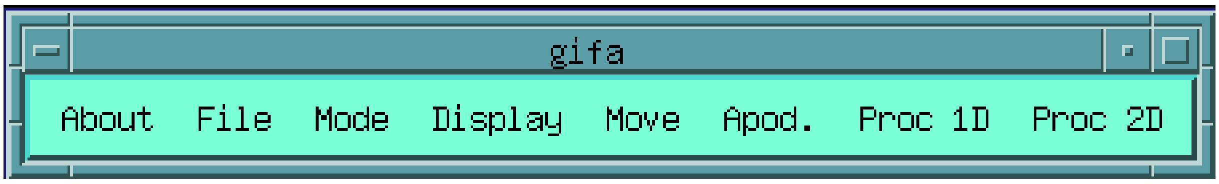
There are five controls to adjust the vertical scale used for displaying the spectra. The Reset button will reset the display to the default, (`ABSMAX 0 SCALE 1`) where the largest peak in the screen in full size. The four other buttons permit to modify the scale value, raising or lowering the SCALE context by factor of 2 and of 1.2. See below for more details on `SCALE`.
The refresh button redraw the spectrum on screen, without changing the settings.
The pop-up menu Dim, can be used to rapidly switch between the 3 working buffers : 1D, 2D and 3D.

Interacting with the mouse

Apart from selecting a zoom window, you can use the mouse to inspect the data. Clicking in the spectral window with the left or the right mouse button, the coordinates (in the currently selected unit) will be displayed in the control box, just below the 1D/2D/3D selector. The intensity of the spectral point at this location is also displayed. If you use the middle button, a cross will also be displayed on the spectrum, permitting to check for peak alignment. When several windows are opened in the same time, the cross lines will extand to all other windows, either 1D or 2D. If the other windows display data coming from different data-set, then lines will be aligned at the same chemical shifts in ppm, regardless of the unit which is currently chosen.
When drawing the zoom box, the coordinates display switched to distance display. This permits to **measure J coupling** or distance between peaks.

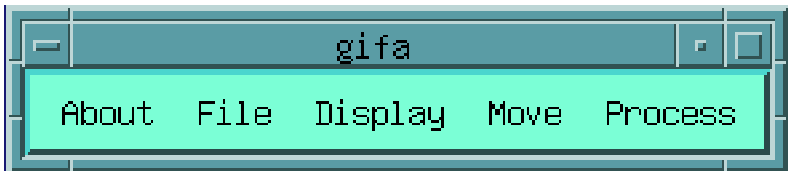
Menu Set-up

The basic-menu graphic user interface is installed in the standard start-up procedure. It is installed whenever the `startup.g` macro is executed. This macro loads the basic environment, and the 1D and 2D processing menus.



The standard menu

An alternate, simplified menu set-up is available, which permits to ease the very first steps in the software. To switch to this simplified setup use the command available in the **About** Menu.



The simplified menu

Note that the menu environment is completely optional, and Gifa can work without any menu bar (even without any graphic window !), or with a completely different graphic environment.

The environment macros are found in the /usr/local/gifa/macro directory. Some macros need additional files for interactive processing or for texts, these files are held into the /usr/local/gifa/macro/gm directory.
There are also sets of related macros, which are put together in sub directories of the main macro directory, for instance 3d processing, assignment, etc...

Basic environment

The following menus are usually present whenever the graphic interface is activated, they are independent from the kind or work currently in progress (except in the assignment module).
If the graphic is missing, try typing the following command `env_base.g`, which executes the macro which loads the default menu-bar, from which you can add all the specific menus.
Some menus are optional or may not be on screen at the same moment, see the **Mode** Menu.
Entries followed by 3 dots (...) indicates that some input will be asked to the user by the command.
The name of the entries in the menus have been chosen to resemble as closely as possible to the command name which would realise the same action. This makes the menus a bit cryptic, but ease the process of learning the commands, which can then be used to extend the capabilities of the program by writing macros. These menus implement most of the actions that you will need in regular processing, however there are many more capabilities in Gifa than the ones which are available from this standard menu interface.

About menu

This menu gives access to the basic information and documentation.

- About GIFA

Will print introduction text, giving the some ideas on the Gifa program, as well as some hints on how getting more information or help.
This button is equivalent to the HELP command without parameter.

- History file

Gives access to the text of the History file.

- Help...

Will prompt you for a command/macro name and will display the help associated with that command/macro.
This button is equivalent to the `help` macro called with a parameter.

- APropos...

Will prompt you for a word, and will show the name of all the commands/macros that have this word in their help file (case insensitive). Try for instance *Fourier* or *display*
This button is equivalent to the apropos macro.

- Documentation...

This button launch the Netscape program, with an hyper-text version of the current manual.

- Gifa home page on the WEB...

This button launch the Netscape program, directly pointing to the Gifa home page :
http://www.cbs.univ-montp1.fr/GIFA/base.html.

- Config

Will give all the details on the internal configuration of the program. You will have information on the current version number and the licence of the program, as well as the value of the basic parameters. Some values are hard-wired in the program at compile time, such as the size of the working buffer, or the number of user variables; some values may be modified by the user such as the kind of plotter currently in use (see below).
This button is equivalent to the CONFIG command.

- bug report

Permits to edit and mail to me Marc-Andre.Delsuc@cbs.univ-montp1.fr a short bug report.

- Switch to Simplified menu

Switch to a simplified mode of the menu environment. This simplified mode is design to help the first time user to use Gifa, concentrating on the most standard features.

- Quit GIFA

Will quit the Gifa program loosing all data in memory not saved with a WRITE command, and

removing the journaling file. If you want to keep the journaling file (a file called gifa.log in your $HOME directory, which holds all the command issued during the Gifa session), you will have to type in the QUIT command directly.
This button is equivalent to the `QUIT N` command.

File menu

This menu holds the basic commands for getting information on the program, reading and writing data-sets and quitting the program.

- Read...

Will prompt you for the name of the file to be loaded into memory. The program will switch to 1D, 2D or 3D depending on the data-set itself. File should be in the standard Gifa format.
This button is equivalent to the READ command.

- Write...

Will prompt you for the name of the file to be written from the data held into memory. The data-set will be created depending on the DIM currently selected (1D, 2D or 3D).
This button is equivalent to the WRITE command.

- Read all format - Write all format

Are equivalent to Read and Write but a selection box permits to choose among all the supported Gifa file formats. For details, see below in the manual at the READx command

- Bring from UXNMR

This button calls an interactive utilities that permits to easily bring data from a remote Bruker spectrometer, and convert it to Gifa data-set.

- Read from VNMR

Calls the macro `varian_read` which makes an interface around the `READV` command, which reads VNMR `FID` files, and the macro `varian_param` which scans the `procpar` file to get acquisition parameters.

- Add file to current

Calls the command `ADD` which permits to add a file to the current data-set (1D, 2D or 3D). A multiplier is used, which permit also to substract, or any other operation.

- File name

Will give you the name of the last read or written file with the `READ` or `WRITE` commands (or the Read... or Write... button).

- Size of data

Will give you the detail on the dimension, the sizes, the spectral widths, etc... of the current data-set. This button is equivalent to the `size` macro.

- More details

Will give you the even more details the current data-set, such as the zoom window, the display values, etc...
This button is equivalent to the `list` macro.

Mode menu

This menu permit to choose between different interface, already prepared in the standard distribution. Some button will completely change the interface, some, noted with 3 leading points, will add a menu at the end of the menu-bar

- Switch to Varian default

After this command has been called, standard processing include a reverse operation, which is suitable for Varian data file, also the `easy2d` form presents an additional entry which permits to directly handle VNMR data files. This is equivalent to using the `Varian` macro

- Proc 1D

Will activate a graphic interface suitable for processing and displaying 1D data-sets only.

- Proc 2D

Will activate a graphic interface suitable for processing and displaying 2D and 1D data-sets.

- Proc 3D

Will activate a graphic interface suitable for processing and displaying 3D, 2D and 1D data-sets.

- Assignment

Will activate the assignment module (see assignment documentation)

- ... Advanced proc

Will add a menu permitting extended processing, such as baseline correction, water suppression, etc...

- ...MaxEnt

Will add a menu permitting to realise MaxEnt processing of the data-sets. (see MaxEnt documentation)

- ...Linear Prediction

Will add a menu permitting Linear Prediction processing. (see Linear Prediction Documentation)

- ...Dosy Processing

Will add a menu permitting Dosy processing. (see Dosy Processing documentation)

- ... Plot

Will add a menu permitting all commands associated to plots.

- ... Peak

Will add a menu permitting all commands associated to Peak-picking and Line fitting.

- ... Unix

Will add a menu permitting Unix-like commands.

- Pulldown menus

Set the menu bar interface to act as a regular pulldown menus. Also resets the interface to 2D Mode

- Static box menus

Set the menu bar interface to act as a set of static button boxes. Also resets the interface to 2D Mode

Display menu

This menu holds the commands permitting to interact with the display.

- Disp1D on

Will switch on the graphic window associated to the 1D buffer. Has no effect if the window is already displayed.

This button is equivalent to the `DISP1D 1` command.

- Disp2D on

Will switch on the graphic window associated to the 2D buffer, displaying the density plot. Has no effect if the window is already displayed.
This button is equivalent to the `DISP2D 1` command.

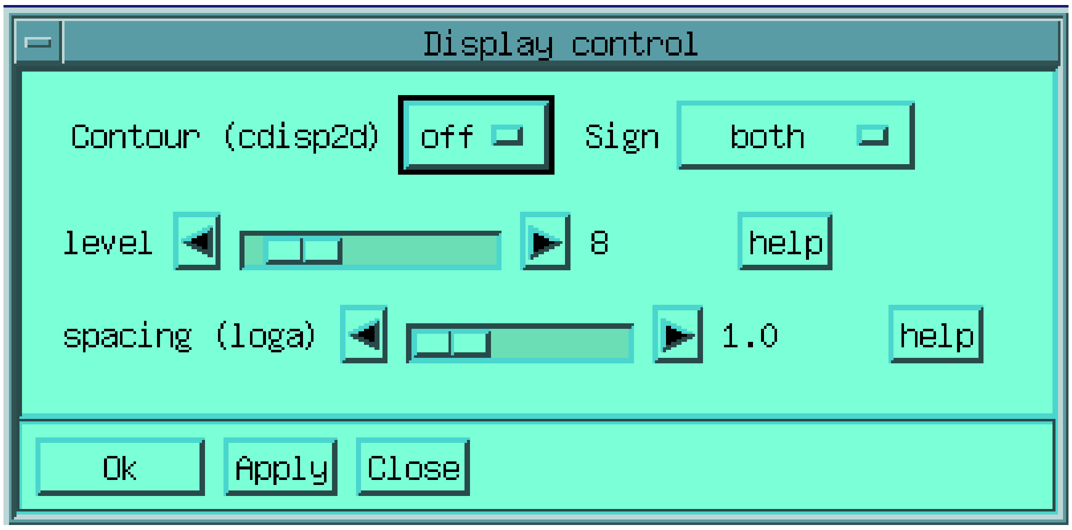
- CDisp2D on

Will switch on the graphic window associated to the 2D buffer, displaying the contour plot. Has no effect if the window is already displayed.
By default when entering the program, the DISP1D and DISP2D windows are on but the CDISP2D window is off. This is because the display in contour plot might be much slower than the density display, and it makes little sense to display a FID in contour plot!
This button is equivalent to the `CDISP2D 1` command.

- Zm (Zoom Control)

This button will enter a Zoom mode, were you can define a zoom window, zoom in and out, and modify the scale of display. The four little arrows permit to move the zoom window around without modifying its size.
This button is equivalent to the `ZM` command.

- Display Control


Display control

Contour (cdisp2d) off Sign both

level 8

spacing (loga) 1.0

This button will launch a form which permits to control other display parameters such as the state of the contour display window, the display of the negative regions, the number of levels and the spacing algorithm.

Equivalent to calling the `dispcont` macro
-sign determines whether positive negative or both levels will be displayed
-level controls the number of levels displayed in the contour 2D window
-loga controls the algorithm used for the level spacing

- Freeze

This button will permit you to "freeze" a currently opened window, by duplicating it. It is a bit like taking a snapshot of the window, letting it on screen as long as you wish. There is no way of altering a FREEZEd window but closing it.
This button is equivalent to the `FREEZE` command.

- Rzoom

When in zoom mode, this button will jump to symmetrical zoom region, relative to the diagonal.
This button is equivalent to the `rzoom` macro.

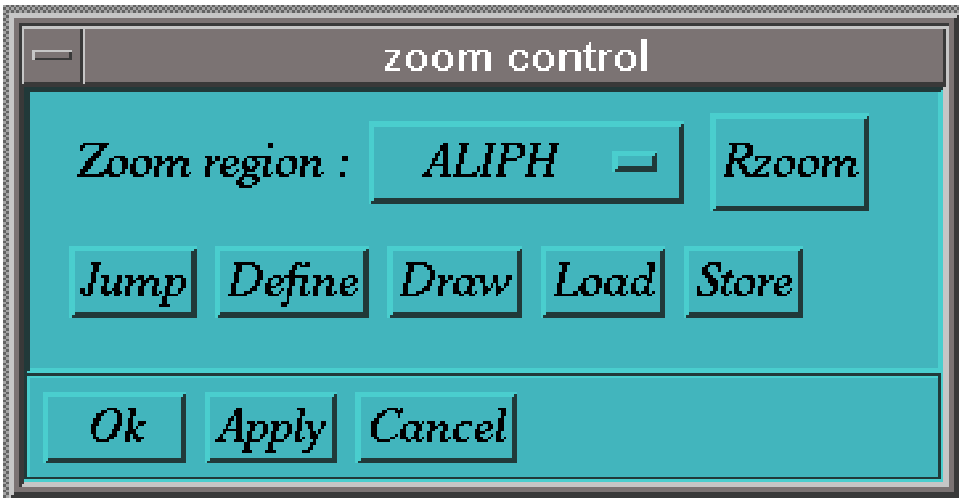
- Store zoom

Clicking this will memorise the current zoom window, it will be possible, at any later time to click on the back to stored zoom to go back to that window.

- Back to stored zoom

Jumps back to the last stored zoom window

- multi_zoom



Brings up a tool which permits to handle several zoom regions easily. Use the pop-up menu to choose the region you want to zoom-in; use the Jump button to actually jump into the selected region; Define permits to define new regions which will appear in the pop-up; Draw draws the defined regions on screen; Load and Store permit to save the configuration to a file call zoom_window. The Rzoom button will do the same action as the command Rzoom above.
This button is equivalent to the multi_zoom macro.

- super1D

Creates a form box which permits to display up to 2 additional 1D spectra on the top of the current 1D spectrum held in memory
Equivalent to the `super1d` macro
Be carefull that this command (as well as super2D) superimposes spectra on the basis of the chemical shift. This permits to compare spectra acquired in very different conditions (spectral width, resolution, even field), but requires that the spectra are correctly calibrated.

- super2D

Creates a form box which permits to display up to 2 additional 2D spectra on the top of the current 2D spectrum held in memory, and displayed on the contour (CDisp2D on) window.
Equivalent to the `super2d` macro

Move menu

This menu holds all the commands permitting to navigate in the different mode of the program, or to move data between the different buffers.
All the processing in Gifa is performed in working buffers. There are 3 main such buffers, the 1D, the 2D and the 3D buffers. The content of the 1D and 2D buffers is directly visualised in the 1D and 2D graphic windows. Only one such working area can be selected at a given time, however switching from one buffer to the other is virtually instantaneous. All commands and actions apply to the currently selected buffer; processing commands (FT, etc..) as well as display commands (`SCALE`, `ZOOM`, etc...). Choosing a working buffer is completely independent from choosing to display one data space or another.

- dim 1 - dim 2 - dim 3

Switches the active working buffer. Respectively to 1D, 2D and 3D. These buttons are equivalent to the `DIM x` command, or to changing DIM from the Zoom Box.

An independent buffer is available, which can hold indifferently a 1D, 2D or 3D data-set. This buffer cannot be easily processed nor visualised, but can be used as an additional "hand" for processing or comparison.

- Put Data

Loads the `DATA` buffer with the contents of the currently active buffer. Equivalent to the `PUT DATA` command.

- Get Data

Brings back the content of the DATA buffer into the working buffer. Equivalent to the `GET DATA` command. The sequence
`Put Data ...any processing... Get Data`
can be used as a kind of limited undo facility. Note however that certain commands use the DATA buffer, thus destroying the Get Data capability.

- AddData

Adds the content of the DATA buffer with the content of the working buffer, and put the result into the working buffer. To make a difference spectra, simply multiply the working buffer by -1 (`mult -1`) before adding. Equivalent to the `ADDDATA` command.

- Point

Enter an interactive mode, where the coordinates of the cursor are displayed. Click into the text box to exit this mode. Equivalent to the `point` macro.

- Unit...

Permits to choose the unit in which the coordinates of the cursor are displayed during the Point mode. Unit can be either Index, Hertz, ppm, second, damping or tabulated. Different unit can be chosen for horizontal and vertical axes in 2D. Equivalent to the `UNIT` and `UNIT_Y` commands.

- Calib...

Starts a macro (`calib`) which permits to calibrate the current spectrum, by clicking on the reference peak, then entering its coordinates.

- Select Row

Starts the macro `rowint`, which permits to interactively select rows (F2 sections) in the 2D window and display them in the 1D window. You exit this mode by clicking on the right mouse button. The last selected row is copied into the 1D working buffer.

- Select Col

Starts the macro `colint`, which permits to interactively select columns (F1 sections) in the 2D window and display them in the 1D window. You exit this mode by clicking on the right mouse button. The last selected column is copied into the 1D working buffer.

- Row...

Permits to copy a 2D row, selected by its index, into the 1D working buffer. Equivalent to the `ROW` command.

- Col...

Permits to copy a 2D column, selected by its index, into the 1D working buffer. Equivalent to the `COL` command.

Processing

These menus permit to perform most of the regular processing to be performed on simple NMR spectra.

Apodisation menu

This menu contains all the operation which are to be applied before the Fourier transform step and is common to all processing modules (1D,2D and 3D), since the apodisation step is the same in all cases. It is installed with the env_proc1d.g macro, along with the Proc 1D menu.

- Em...

Apply an exponential apodisation to the current data-set. The value of the exponential is in Hertz. There is one parameter for each axis in the data-set (1 in 1D, 2 in 2D, 3 in 3D). Equivalent to the `EM` command.

- Gm...

Apply an Gaussian apodisation to the current data-set. The value of the Gaussian is in Hertz. There is one parameter for each axis in the data-set (1 in 1D, 2 in 2D, 3 in 3D). Equivalent to the `GM` command.

- Sin...

Apply a sine-bell apodisation to the current data-set. The first (and only in 1D) parameter is a value ranging from 0.0 to 0.5; the value of the parameter corresponds to the position of the maximum of the filter in your window, thus 0.0 is pure cosine, 0.5 is pure sine, all intermediate values are possible. In

2D or 3D you will be prompted for the axis on which the apodisation should be applied.
Equivalent to the `SIN` command.

- SqSin...

As the Sin button but applies a squared sine-bell. Equivalent to the `SQSIN` command.

- Tm...

Applies a trapezoidal apodisation. You will be prompted for two parameters, the built function starts from 0.0, raises up to the index entered as the first parameters where it reaches 1.0, the decay from 1.0 to 0.0 starts a the index entered as the second parameter up to the end of the data-set. In 2D or 3D you will be prompted for the axis on which the apodisation should be applied. Equivalent to the `TM` command.

- Gaussian Interactive

Permits to interactively use a Gaussian resolution enhancement, by combining a Gaussian apodisation and an exponential one. Equivalent to the `gm_inter` macro.

- User defined...

Applies an apodisation which can be defined as an equation by the user. Equivalent to the `user_apod` macro.

- Correct 1st point

Correct the first point of the current data set for the quantification bias introduced by the sampling. This is typical correction on 2D-3D data-sets. It partially removes the *t1-ridges* that are commonly seen. It has less interest in 1D.

- ChSize...

Permits to change the size of the current data-set. The operation (reduction or increase) will be realised at once on the data-set. Increasing the size will be realised by adding zeros at the end of the buffer. You will be prompted for a dimension per axis in the data-set.
Equivalent to the `CHSIZE` command.

Proc 1D menu

This menu, installed with the env_proc1d.g macro, holds the commands for 1D processing.

- Easy1d

This command opens a form permitting to rapidely process a 1D experiment.You select the size, the apodisation function, the Fourier, phasing and Baseline correction steps. The set-up can be used for direct computation as well as to store a macro that will realise the process in a latter stage. See the details in the chapter Basic (1D) Processing Check also the on-line help

- ZeroFill

Extend the size of the current data-set to a size equal to the next power of two. This is realised with the `CHSIZE` command.

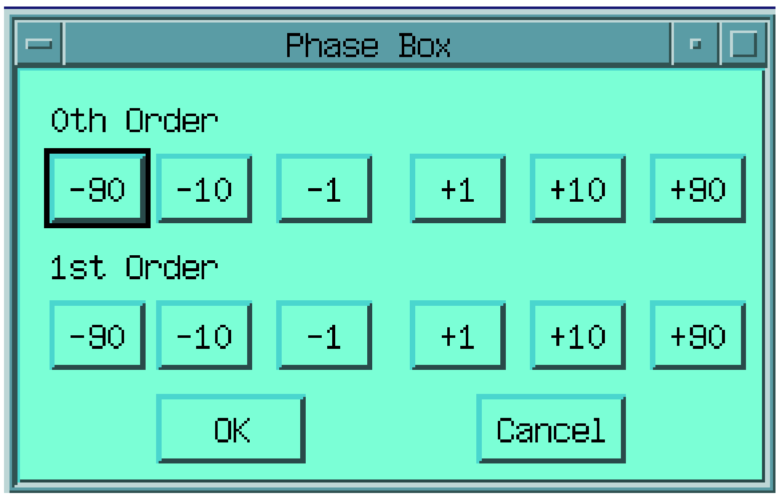
- ft_Seq

Realises the Fourier transform suitable for a data set acquired in *sequential* mode : real and imaginary part alternatively sampled. Equivalent to the `ft_seq` macro or to the `REVF RFT` command.

- ft_Sim

Realises the Fourier transform suitable for a data set acquired in *simultaneous* mode : real and imaginary part sampled at the same time point, and stored alternatively in the buffer. Equivalent to the `ft_sim` macro or to the `REVF FT` command.

- Ph



Starts the `PH` command which permits to interactively phase the current spectrum. Pops up a control graphic box, which permits to control zeroth and first order phase corrections, place the pivot (with the middle button of the mouse), and store the phase correction. Zoom and the Zoom Box controls are still active.

- Auto. Phasing

Computes a phase correction on the current 1D data-set, using the APSL techniques (A.Heuer J.Magn.Reson. 91 p241 (1991)). This is equivalent to calling the `apsl` macro.

- Redo Phase

Apply to the data-set the last phase correction used. Equivalent to the `PHASE %%` command.

- Real

Remove the imaginary part of the data-set, thus reducing by two the number of buffer points.

Equivalent to the `REAL` command.

- Modulus

Compute the modulus of the spectrum from the real and imaginary parts. Equivalent to the `MODULUS` command.

- Integrate

Start the 1D graphic integration module.
See Basic (1D) Processing for details.

Proc 2D menu

This menu, installed with the env_proc2d.g macro, holds the commands for 2D processing. The F1 axis always refers to the non-classical, vertical axis of the 2D, and the F2 axis to the classical, horizontal axis. Some commands are specific to F1 or F2 processing, some commands prompt for the axis to process, in which case you have to enter either F1, F2 or F12 if you want a processing on both axes.

- Easy 2D

This button launches a form which simplifies the Fourier transform process. You select the sizes, the apodisation functions, the Fourier, phasing and Baseline correction steps. The set-up can be used for direct computation as well as to store a macro that will realise the process in a latter stage. See the details in the chapter Handling of 2D and 3D Data-sets Check also the on-line help.

- ZeroFill F1 - ZeroFill F2

Increases the size of the dataset in the F1 or F2 domain up to the next power of 2. performed with the `CHSIZE` command

- Burg 2D

This button permits to use the burg Linear prediction method for extending the data-set. You can see it like a sophisticated zero-filling function. Equivalent to the `burg2d` macro.

- Svd 2D

This button permits to use the Linear prediction method for extending the data-set. The LP method used here is based on the computation of a singular value decomposition (SVD) from each row of the data-set. It is more sophisticated, but much slower than the Burg method.

- ft_Seq (F2)

Realises the Fourier transform in F2 suitable for a data set acquired in *sequential* mode : real and imaginary part alternatively sampled. Equivalent to the `ft_seq` macro or to the `REVF F2 RFT F2` command.

- ft_Sim (F2)

Realises the Fourier transform in F2 suitable for a data set acquired in *simultaneous* mode : real and imaginary part sampled same time point, and stored alternatively in the buffer. Equivalent to the `ft_sim` macro or to the `REVF F2 FT F2` command.

- ft_phase_modu (F1)

Realises the Fourier transform in F1 suitable for a data set acquired in phase modulation mode. Equivalent to the `ft_phase_modu` macro or to the `FLIP REVF F1 FT F1 FLOP` command.

- ft_tppi (F1)

Realises the Fourier transform in F1 suitable for a data set acquired in TPPI mode. Equivalent to the `ft_tppi` macro or to the `RFT F1` command.

- ft_sh (F1)

Realises the Fourier transform in F1 suitable for a data set acquired in Hypercomplex (States-Haberkorn) mode. Equivalent to the `ft_sh` macro or to the `REVF F1 FT F1` command.

- ft_sh_tppi (F1)

Realises the Fourier transform in F1 suitable for a data set acquired in TPPI Hypercomplex (TPPI States-Haberkorn) mode. Equivalent to the `ft_sh_tppi` macro or to the `FT F1` command.

- ft_n+p (F1)

Realises the Fourier transform in F1 suitable for a data set acquired in echo-antiecho mode, with alternated gradients. Equivalent to the `ft_n+p` macro.

- Ph in f1 (ph2dc)

Starts the macro `ph2dc` which permits to interactively phase a 2D spectrum in F1. You first enter a selection mode, where you click on the 2D window with the left button to visualise the columns, you select them with the middle button, the selected columns are added together. You exit this mode with the right button. You then enter the `PH` command with a composite 1D spectrum obtained from the selected columns. The phase obtained on this spectrum is then applied on the complete 2D.

- Ph in f2 (ph2dr)

Equivalent to `ph2dc` for the F2 domain.

- Redo Phase F1

Apply again the last phase correction in the F1 domain. Equivalent to the `PHASE % % F1` command

- Redo Phase F2

Apply again the last phase correction in the F2 domain. Equivalent to the `PHASE % % F2` command

- Real F12

Remove the imaginary parts of the data-set along each axis, thus reducing the total size of the data-set by four. Equivalent to the `REAL F12` command.

- Modulus

Computes the modulus spectrum from the real and imaginary parts. Equivalent to the `MODULUS` command.

- Proj F1

Computes the projection of the 2D dataset along the F1 axis, onto the F2 axis. The command will prompt you whether you want a "Skyline" (keep the highest points) or a "Mean" (sum all points) projection. Equivalent to the PROJ F1 command.

- Proj F2

Computes the projection of the 2D dataset along the F2 axis, onto the F1 axis. The command will prompt you whether you want a "Skyline" (keep the highest points) or a "Mean" (sum all points) projection. Equivalent to the PROJ F2 command.

- Proj_loc

Computes a local projection of the 2D dataset along any chosen axis, the projection is computed from only a part of the data-set, by default you are prompted for the current zoom window.

- ...2D on file

This menu entry adds an additionnal menu called '2D on file' which ease the process of processing very large 2D, working on file rather than in memory. With this set-up there is no limit on the size of the 2D that can be processed. see Working On File rather than In Memory for details.

The equivalent command is : `env_2donfile.g`

2D on file

When a data-set is too big to be processed in-memory, it is possible to realize the processing on-file. This is done with a special set-up in Gifa, the "cache" system, which permits to access files in an optimal fashion, (see below the Working On File rather than In Memory chapter).
This mode is rather designed for 3D processing, however it is perfectly possible to handle 2D in this way. 2D processing on file is done by having an input file and an output file, planes are loaded from the input file, processed in memory as regular 1D experiment, and then copied on the output file.

- Join data-set...

This entry permits to realize the first operation to be done, namely connecting to the input file. This is equivalent to the `JOIN` command. Once a data-set has been JOINed, it is possible to display internal parameters, load 1D from it, or load a 2D region form it. Note that you can issue that command to several files, thus being JOINed to more than one file. However all the command will refer to the last JOINed file.

- Dataset parameters

That button simply runs the `dataset` macro, which displays all the spectral parameters of the current JOINed data-set. Note that since the header holding all the parameters is in ASCII format, one can simply make `more filename` to see the value of all the parameters.

- list all files

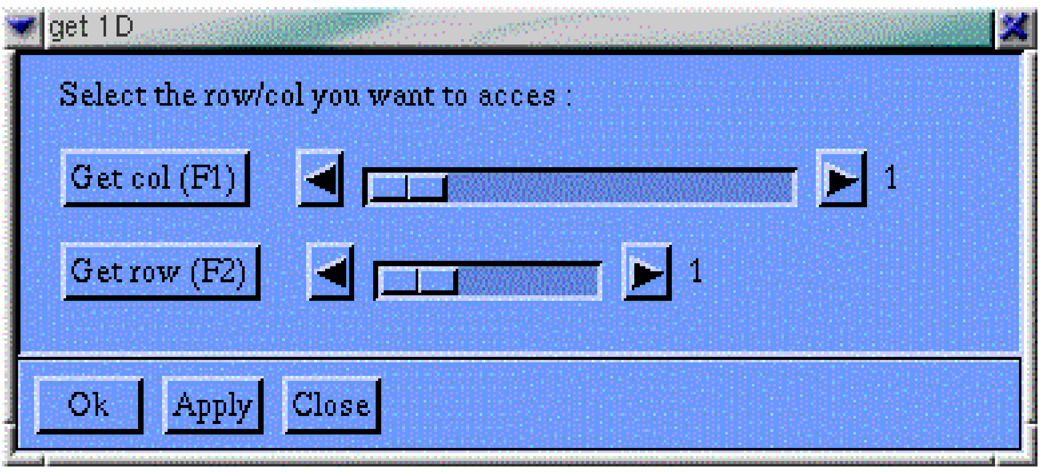
This button lists the names of all the files which are currently JOINed.

- disjoin

Once a file have been JOINed it must be DISJOINed in order to release completely the internal memory.

- get 1D

This menu entry permits to load a 1D plane extracted from the currently JOINed 2D dataset. A graphic box is displayed :



get 1D

Select the row/col you want to acces :

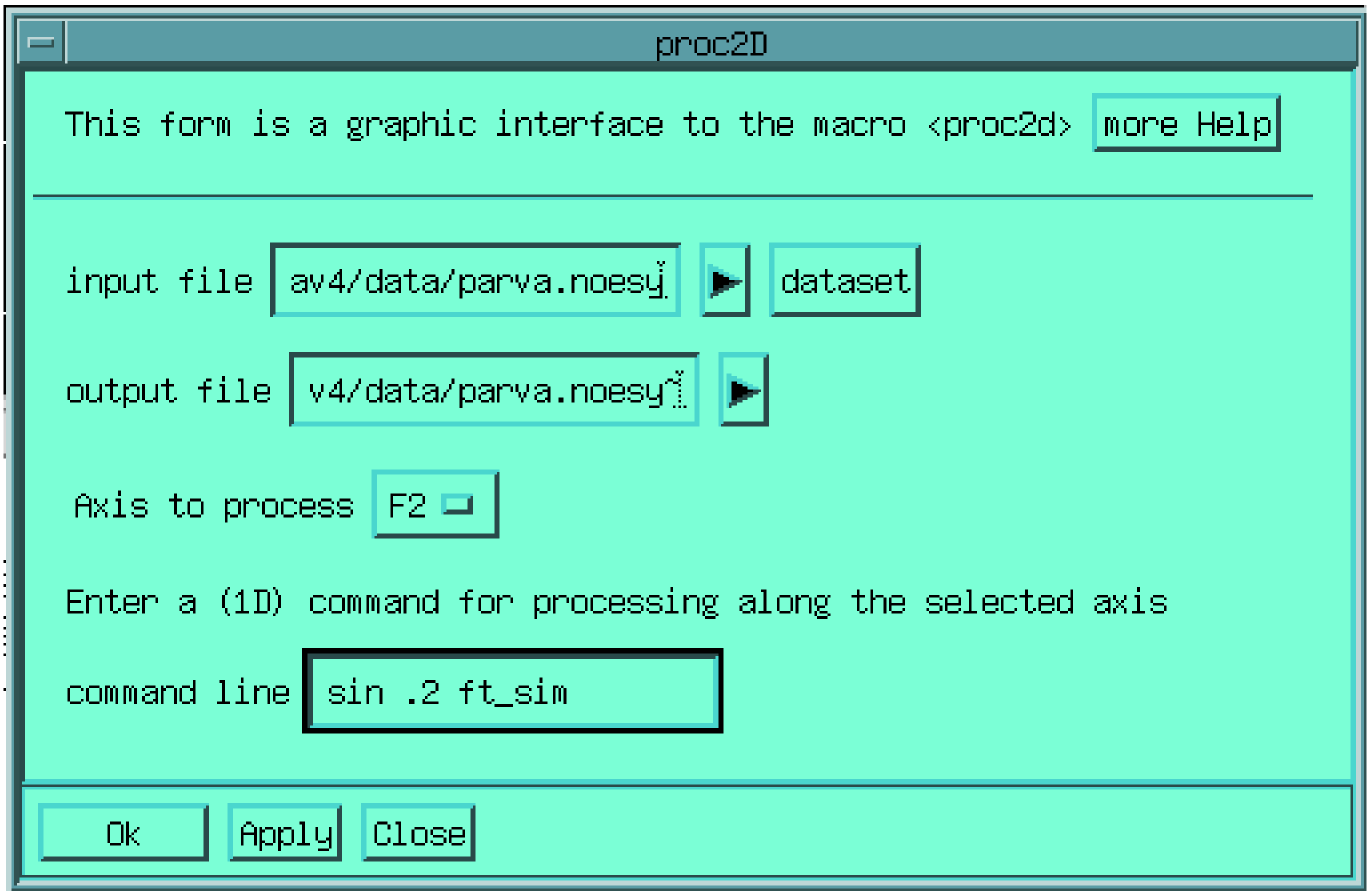
Which permits to rapidely select row and columns from the experiment.
For instance it can useful to load the first F1 or F2 Fid to determines the optimum processing parameters, and phases, before going to full 2D processing. It is equivalent to using the `GETC` command in `DIM 1` mode.

- get region

This ones permits to load in the central memory a portion of the currently JOINed data-set. You will be prompted for the coordinates fits point (F1, F2) and then for the coordinates of the last point (F1, F2). It is equivalent to using the `GETC` command in `DIM 2` mode.

- 2D proc...

This button creates a form which permits to process the 2D data-set on-file. One has to enter the name of the input and output files, the axis along which the processing will be done, and finally the command line that will be applied to each plane of the 2D.



proc2D

This form is a graphic interface to the macro <proc2d>

input file av4/data/parva.noesy

output file v4/data/parva.noesy

Axis to process F2

Enter a (1D) command for processing along the selected axis

command line sin .2 ft_sim

This command line will be executed in 1D mode on each of the planes; thus typical 1D command should be given here. The forms actually calls the `proc2d` macro.

- Proj F1 ...
- Proj F2 ...

Compute the projection plane along the corresponding axis. You will get prompted for the projection mode Skyline / Mean

---

3D menus

When 3D processing has been chosen, either with the env_proc23d.g macro, or the Proc 3D option in the **Mode menu,** 3 additional menus are inserted in the menu bar. The first menu is for processing 3D data-sets which can be held into the central memory, the second is specific of 3D display, and the third one is for processing and displaying file which are too big for fitting into the central memory, and thus have to be processed on file.
In 3D processing F3 axis always refer to the acquisition axis, F1 refers to the axis which is stored with the slowest increment, and F2 to the intermediate axis. Thus, 3D can be seen a series of F2-F3 planes. Note that this definition depends only on how the data-set was stored, and not on the order of the incremented delays in the sequence.
Naming of planes is done by giving the axis orthogonal to the plane rather than the axes in the planes; for instance the planes holding the F1 and F3 planes are noted F2 planes.

Proc 3D

This menu holds most of the commands for processing 3D experiments in-memory, as it is done for 2Ds. This can be done only for not too big data-sets. In the contrary case, one has to resort to on-file processing (see below). The Gifa central memory is determined at compile time, and several versions of the program, corresponding to different size of the memory, should be available on your machine, check the installation manual.
In the case of in-memory processing, commands are very similar to what is done in 2D.

- Largest Set

This button simply call the `largest_3d` macro which gives you example of data-sets which fit into the memory.

- ZeroFill F1

Simply realizes extension of the size in F1, to the next power of two. Done with the `CHSIZE` command.

- ZeroFill F2

Realizes extension of the size in F2, to the next power of two. Done with the `CHSIZE` command.

- ZeroFill F3

Realizes extension of the size in F2, to the next power of two. Done with the `CHSIZE` command.

- Burg3d

Performs the burg extension of the data-set in F1 or F2 using the `burg3d` macro command.

- ft_Seq (F3)

Performs in the F3 (acquisition) axis, the Fourier transform of a data-set acquired in *sequential* mode.

- ft_Sim (F3)

Performs in the F3 (acquisition) axis, the Fourier transform of a data-set acquired in *simultaneous (complex)* mode.

- ft_tppi (F2)
- ft_sh (F2)
- ft_sh_tppi (F2)
- ft_tppi (F1)
- ft_sh (F1)
- ft_sh_tppi (F1)

Performs in the F2 or F1 axis, the Fourier transform suitable for data-sets acquired with different protocols, see the **Proc 2D** menu for details.

- Phase

Permits to apply a phase correction in a given spectral axis. Equivalent to the `PHASE` command.

- Real...

Permits to throw away the imaginary part associated with a given axis (F1, F2 or F3). Equivalent to the

`REAL` command

- Real F123

Permits to throw away all the imaginary part associated to a fully hypercomplex data-set. Equivalent to the `REAL F123` command.

- Modulus

Computes the modulus of fully hypercomplex data-set. Equivalent to the `MODULUS` command.

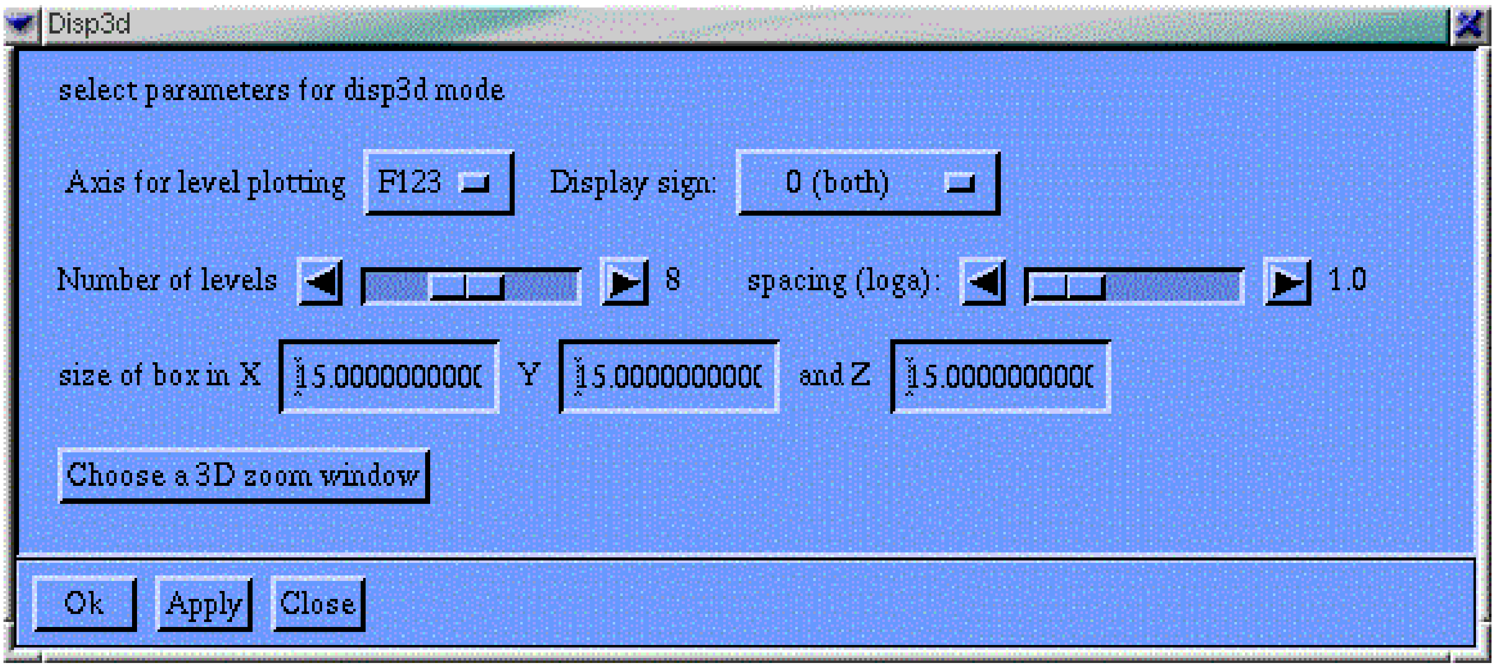
Display 3D

This menu holds all the functions for displaying the 3D data-set held into memory

- disp3d on

Opens the 3D display window, equivalent to the `DISP3D 1` command.

- parameters...


Disp3d

select parameters for disp3d mode

Axis for level plotting: F123 — Display sign: 0 (both)

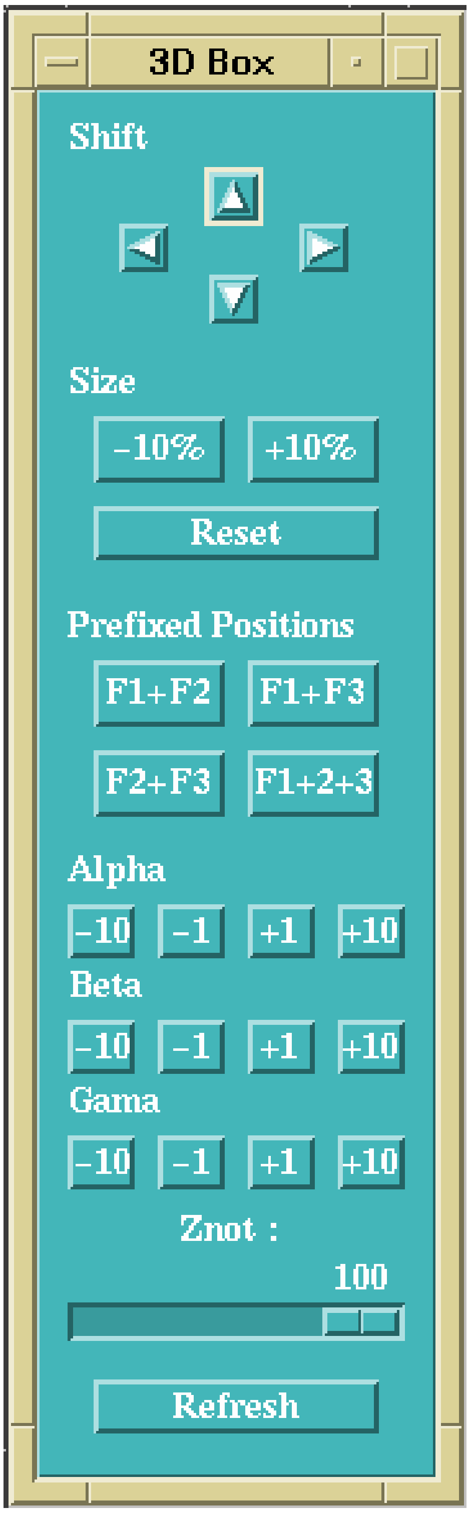
Number of levels: 8 — spacing (loga): 1.0

size of box in X: 15.000000000(— Y: 15.000000000(— and Z: 15.000000000(

Opens a form for setting 3D display parameters. actually calls the `disp3d_form` macro.

Axis for level plotting determines along which axes (F1, F2, F3 or combinaitions) the contour will be plotted
Display sign determines wether only positive or negative levels should be displayed
Number of levels and spacing are standard 2D contour plot parameters (see LEVEL or LOGA)
Size of box determines the CX, CY and CZ parameters
Choose a zoom window starts a utility helping in defining the 3D zoom window

- control box



Opens a control box which permit to interactively chose the view point of the 3D display. Equivalent to the `CHECK3D 1` command.

This control box permits to change its position and size within the window, to set the orientation of the spectral cube, to change the perspective of the display, and finally to recompute a display with the Refresh button.
refresh
In contrast with the other windows, the 3D display is not automatically refreshed whenever a display parameter changes. This has been chosen because of the time that this refresh might take. Clicking on this button will start the 3D display. Equivalent to the `REF3D` command, or to the *Refresh* button on the CHECK3D control box.

- choose zoom...

This button starts the `zoom3di` macro which permits to interactively choose a zoom window for the current 3D display.

- plane...

Calls the `PLANE` command, which loads the 2D buffer with a plane extracted from the 3D.

- diag...

Calls the `DIAG` command, which loads the 2D buffer with a diagonal plane extracted from the 3D

- vertint

Starts the `vertint` macro which permits to interactively examine 1D spectra by clicking on a orthogonal 2D plane.

- planeint

Starts the `planeint` macro which permits to interactively examine planes by clicking on a orthogonal 1D spectrum

- Proj F1 ...

- Proj F2 ...

- Proj F3 ...

Compute the projection plane along the corresponding axis. You will get prompted for the projection mode Skyline / Mean.

3D on file

When a data-set is too big to be processed in-memory, it is possible to realize the processing on-file. This is done with a special set-up in Gifa, the "cache" system, which permits to access files in an optimal fashion, (see below Working On File rather than In Memory chapter).
3D processing on file is done by having an input file and an output file, planes are loaded from the input file, processed in memory as regular 2D experiment, and then copied on the output file.

- Easy 3D

This button launches a form which simplifies the 3D processing. Each step is detailled through a 2D processing step, using easy2d. The set-up can then be used for direct computation as well as to store a macro that will realise the process in a latter stage. See the details in the chapter Handling of 2D and 3D Data-sets Check also the on-line help.

- Join data-set...

This entry permits to realize the first operation to be done, namely connecting to the input file. This is equivalent to the `JOIN` command. Once a data-set has been JOINed, it is possible to display internal parameters, load 1D or 2D from it, or even load a 3D region form it. Note that you can issue that command to several files, thus being JOINed to more than one file. However all the command will refer to the last JOINed file.

- Dataset parameters

That button simply runs the `dataset` macro, which displays all the spectral parameters of the current JOINed data-set. Note that since the header holding all the parameters is in ASCII format, one can simply make `more filename` to see the value of all the parameters.

- list all files

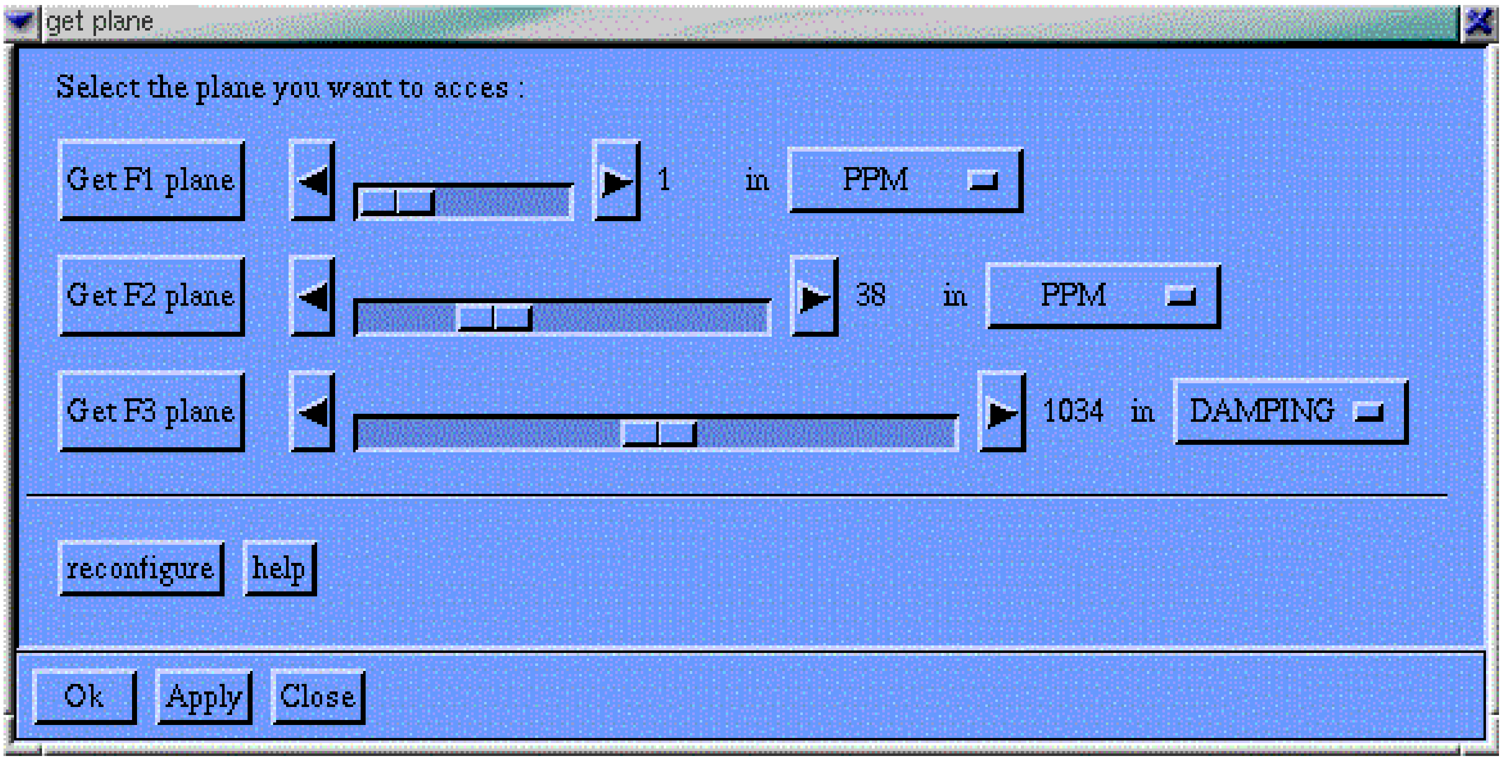
This button lists the names of all the files which are currently JOINed.

- disjoin

Once a file have been JOINed it must be DISJOINed in order to release completely the internal memory.

- get plane

This menu entry permits to load a plane extracted from the currently JOINed 3D dataset. For instance it can useful to load the first F1 or F2 planes to determines the optimum processing parameters, and phases, before going to full 3D processing. It can used also to look at planes in a processed data-set. It is equivalent to using the `GETC` command in `DIM 2` mode.



Select the plane you want to acces :

1 in PPM

38 in PPM

1034 in DAMPING

The box permit to access directly planes along the 3 axes. You can choose planes in index as well as in PPP or Hz. Hit reconfigure when changing the unit to be used along one axis.

get region

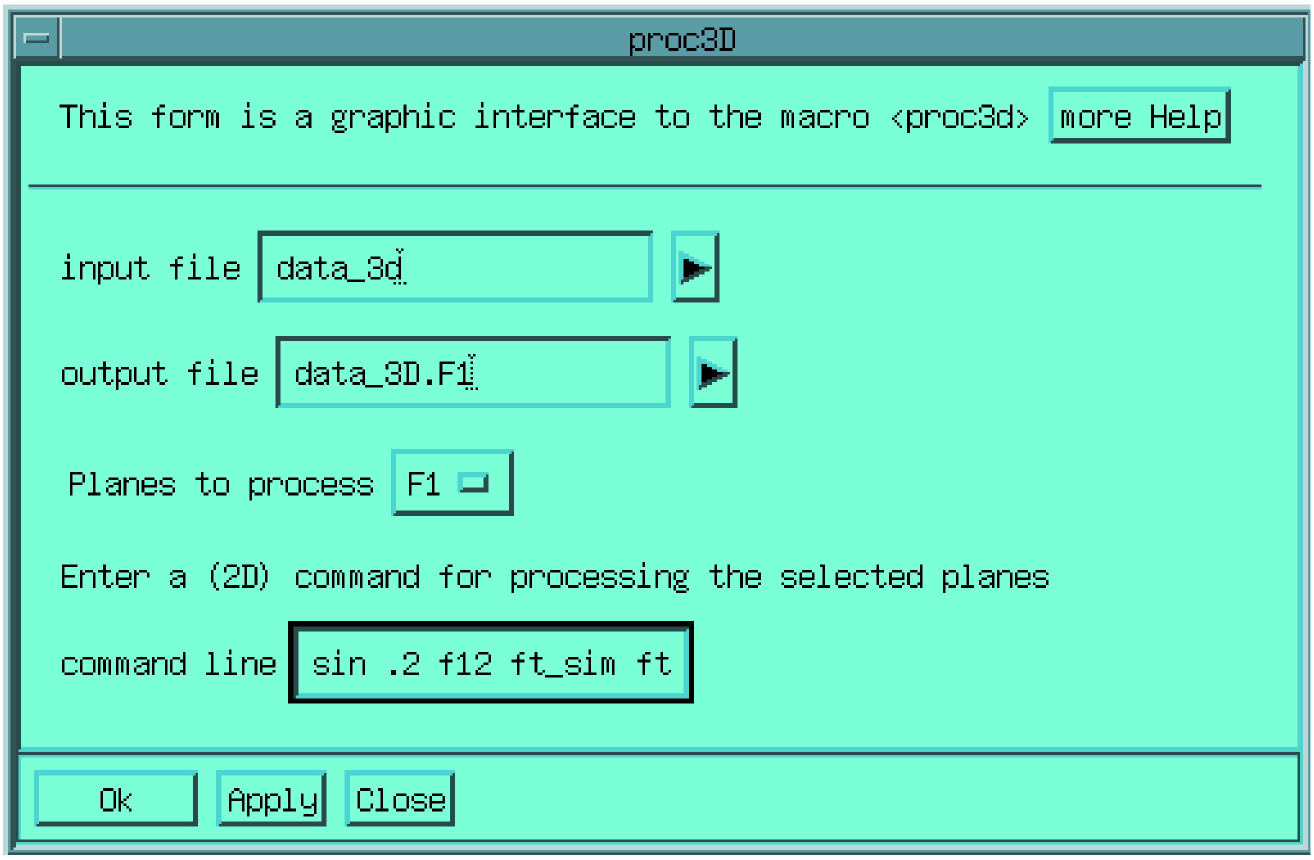
This ones permits to load in the central memory a portion of the currently JOINed data-set. You will be prompted for the coordinates fits point (F1, F2, F3) and then for the coordinates of the last point (F1, F2, F3). It is equivalent to using the `GETC` command in `DIM 3` mode.

- get vertical

After having loaded a 2D plane from the currently JOINed 3D, you can acces 1D 'verticals' with this command. Simply clicking in the 2D plane brings the 1D line in the 1D window.

- 3D proc...

This button creates a form which permits to process the 3D data-set on-file. One has to enter the name of the input and output files, the axis along which the processing will be done, and finally the command line that will be applied to each plane of the 3D. This command line will be executed in 2D mode on each of the planes; thus typical 2D command should be given here.


proc3D

This form is a graphic interface to the macro <proc3d>

input file: data_3d

output file: data_3D.F1

Planes to process: F1

Enter a (2D) command for processing the selected planes

command line: sin .2 f12 ft_sim ft

The forms actually calls the `proc3d` macro.
Proj F1 ...

- Proj F2 ...

- Proj F3 ...

Compute the projection plane along the corresponding axis. You will get prompted for the projection mode Skyline / Mean

- Compute all Proj

Compute the three projection planes along the three corresponding axis, and put the result in the first planes of each axis. Thus the (say) F1 projection is found has the first plane in F1. This command has to be done only once on the data-set.

- strip_file

Construct a strip plot from the current 3D and load it into the 2D buffer. Uses the currently JOINed 3D and the content of the 2D peak table.

- strip_plot

Construct a strip plot from the current 3D and send it to a plot file. Permits to plot on several pages. Uses the currently JOINed 3D and the content of the 2D peak table.

Optional menus

The following optional menus can be accessed from the **Mode** menu.

Advanced proc menu

- BCorr linear

Apply a linear baseline correction to the current data-set. You have to click on empty regions of the data-set, from which the baseline correction will be computed. Equivalent to the `point` and `BCORR 1` commands.

- BCorr Spline

Apply a spline baseline correction to the current data-set. You have to click on empty regions of the data-set, from which the baseline correction will be computed. Equivalent to the `point` and `BCORR 2` commands.

- BCorr Polyn.

Apply an automatic peak detection followed by a polynomial baseline correction. Equivalent to the `BCORR 3` command.

- 1D Hilbert

Realises the 1D Hilbert transform of the current data-set, that is the current real data-set is transformed to a complex data-set with a reconstructed imaginary part. The operation is done without changing the total number of data points. Is equivalent to

```
IFTBIS FT
```

- 1D invHilb

Realises the 1D inverse Hilbert transform of the current data-set, that is the current complex data-set is transformed to a real data-set with all the information of the imaginary part brought back to the real region. The operation is done without changing the total number of data points. Is equivalent to

```
IFT CHSIZE(%*2) FT REAL
or
IFT FTBIS ; better
```

- 2d Hilbertsxx and 2DinvHilb xx

These menus realises the direct and inverse Hilbert transform of the 2D data-set.

- DMX phase

When an FID comes from a digitally filtered DMX spectrometer, a dramatic phase corection as to be applied. This command uses the value of DECIM (found in the `acqus` file) to compute a phase correction of the current 1D or 2D spectrum. To be applied on a SPECTRUM.

- DMX phase

Applies a phase correction correction suitable to restore DMX dataset. The phase correction is obtained from DECIM. To be applied on a spectrum.

- DMX clean

Uses the phase correction obtained from DECIM to correct the FID and generate a causal FID, using the Hilbert transform. To be applied on a FID

- Remove H2O

Starts the `rem_h2o` macro which remove substantially solvent signal at zero frequency in the FID. It does so by removing any slow varying signal in the FID, using the baseline correction module. Should be applied on the time-domain data-set, before any other processing (before apodisation or Fourier transform).

MaxEnt menu

This menu holds some commands than permit to simply process a 1D or 2D data-set using Maximum Entropy deconvolution. The menus are more or less organised in the order in which you should use them.
You should start with a spectrum, phased, baseline corrected, but, ideally, not apodised. You can do processing from an apodised data-set but you will get better results if you start over with a spectrum obtained without any apodisation.
Using this menu, Maximum Entropy can only be applied on a spectrum containing only positive, absorptive spectra.
For a complete understanding of MaxEnt processing, read that part of the manual devoted to MaxEnt.

- Prepare Data

With this command you first select a small region of the spectrum that you wish to process. You should not use a complete spectrum, but rather concentrate on the interest region with this command. The command also realizes the inverse Fourier transform step which is necessary to create the pseudo-FID that will be used later on by MaxEnt.

- Eval Noise...

Before running the process you should determine the noise quantity present in the pseudo-FID by zooming, with this command, on the end of FID holding only noise. If the starting data-set had been apodised, the noise quantity will be largely under-estimated; if the pseudo-FID is truncated (total decay is not obtained), the noise quantity will be overestimated. In any case you may want to correct it with the `NOISE` command.

- Deconvolution fct...

Before running the process you should determine the deconvolution function, which can be either Lorentzian or Gaussian (other possibility are available from the command level). Line-width is entered in Hz. The line-shape thus defined will be removed from the actual spectrum, thus producing sharer lines. So you should never enter here a line-shape larger than the sharper line present in the spectrum.

- Iterations...

Determines the number of iterations that will be used for the starting computation.

- Start Iteration

Starts the MaxEnt iterations. You are first prompted for the size of the spectrum to be computed, which should larger or equal to the size of the pseudo-FID. Never starts the computation if
¥ you don't have a FID on screen
¥ you don't have realised the previous steps
During the iterations you should check the following values : *chi2*, should be as small as possible, *chi2* = 1 means the computation is finished; *conv* should be as small as possible, a *conv* larger than 0.1

means that the convergence will never be obtained, probably because the data-set or the deconvolution function are incorrectly chosen.

- 10 more

Continue the processing for 10 more iterations.

- Restart

Start over the processing with the pseudo-FID.

- remove background...

When the computation is completely finished, you should remove the background that MaxEnt always adds to the spectrum, by running this command and zooming in an empty region of the spectrum. After this operation, the process should be started over. (10 more is not available any more)

Linear Prediction menu

This menu holds all the entries for realising simple Linear prediction calculations. (still experimental - the menu I mean, the commands are fully operational)
To fully understand what is going on here, you are supposed to have read the manual (no joking :-).
Most (all ?) entries here, are supposed to be applied on untouched (i.e. not apodised) FID.
This menu is built by the env_lin_pred.g macro.

- Order

Permits to determine the value of ORDER used for all LP operation. Should be set larger than the number of lines in the spectrum, and smaller than the data-set size. The speed of LP operations usually depend on this setting.(see LP documentation). Equivalent to the ORDER command.

- make FID Cplx

LP commands work only on Complex FIDs, this button transform a Real FID into a Complex one by using a Hilbert transform. Equivalent to the command `IFTBIS FT`

- burg extension

Extend the current FID using the burg method. Can be used to correct truncated FID. To be used BEFORE any apodisation. Will prompt you for the new size.
Equivalent to using the BURG command, or the `dt->ar ar->dt` *`size`* `1` sequence.

- SVD extension

Is equivalent to the previous button, but uses the SVD method which is somewhat slower, but more efficient in the case of noisy data. Try this one if burg failed. Equivalent to using the `dt->svd % svd->ar 1 ar->dt` *`size`* `1` sequence

- stable SVD extension

Equivalent to the precedent, but even slower. That one should succeed in all cases. To be used when the previous one failed (typically by transforming your FID into "trumpets" (increasing exponentially towards the end))
Equivalent to using the `dt->svd % svd->ar 1 ar->rt 1 rtreflect 1 rt->ar 1 ar->dt` *`size`* `1` sequence

- burg 1st points

Uses the burg method to build missing first points. Can be used for instance after a lshift to correct for acoustic ringing.
It is the burg_rev macro

- SVD 1st points

Equivalent to the previous, but with the SVD method. It is the svd_rev macro.

- burg spectrum

Computes the "Burg spectrum" (also called mem1) i.e. an estimate of the power spectrum, based on the burg analysis of the FID.
Prompts you for a size on which the spectrum should be recomputed.

- SVD analysis

Performs a complete SVD analysis of the current FID. Results are put into the pklist

- FAB-SVD analysis

The same as previous, but uses the *Forward & Backward* method. Meant to be used on very bas signal/noise cases.
Will prompt you for an exact number of line to keep in the spectrum.

- Cadzow proc.

Applies the Cadzow procedure to clean up the current FID. Calls the Cadzow macro.

- PKlist

Actually prints the content of the peak table. Equivalent to the pklist %% macro.

Plot menu

This menu holds all the entries for realising simple plots.

- Easy plot

This button launches a form which permits to determine all the parameters for a standard plot, with axes, grid, choice of colours, etc... See the details in the chapter Plotting

- Plot...

Starts the macro plot? which prompts you for some basic parameters associated to plotting : the kind of plotter (postscript or HP-GL), the size of the plot in centimetres, the offset of the plot from the lower left corner of the page, the vertical offset of 1D plots, the rotate state and the parameters for spectral axes. Can be used to pre-set the values in Easy Plot

The other menu entries permit to realise more specific plots. Each entry add a element to the current plot, and the final entry Page send this plot to the plotter.

- Screen Dump

Adds the current display (1D or 2D) to the plot.

- Title

Adds a title to the current page. When entering more than one word, put the complete string into quotes (') or double quotes (").

- Plotaxis F1 - Plotaxis F2

Add an labelled axes on the F1 (y) or F2 (x) direction, as defined with the Plot? command.

- Grid F1 - Grid F2

Add a grid in the F1 or F2 domain according to the definition of the axis from Plot? command.

- Page

Send the current plot to the plotter. On certain platform, the plot file is displayed on screen before being actually sent.

- Cindy...

Makes a plot file which can then be read with the NMR analysis Cindy program (see ftp://www.cbs.univ-montp1.fr/pub/Cindy). Equivalent to the `FPLOT` command.

Peaks menu

This menu holds certain facilities for realising peak detection, peak integration and line fitting. All the information is held into an internal table which can be displayed at any time with the PKLIST button.

- eval noise

Asks you to zoom on an empty region, and evaluates noise on the selected region. Uses the `EVALN` command..

- Peak sign

Permit to choose whether the peak picker will search for positive or negative peaks.

- Peak pick

Enter the macro `pp` which performs a simple peak-picking. You should have evaluated the noise level with the previous button Then zoom on the region to be peak-picked. The peak threshold is evaluated from the noise level.

- add peaks

Permits to add a peak into the table by clicking on the data-set. Equivalent to the `point POINT->PK` command.

- rem peak

Calls the `pkrmi` macro which permits to interactively remove a peak on the data-set.

- rem peaks

Calls the `pkrmz` macro which permits to interactively remove a set of peaks on the data-set.

- pkclear

Equivalent to the PKCLEAR command, which removes all peak entries.

- rem peaks along diagonal

Calls the `pkrm_diag` macro which removes all peaks within a given distance from the diagonal of a homonuclear experiment

- peak symmetrise

Calls the `PKSYM` command, which "symmetrises" the 2D peak table, you can either remove all peaks with no symmetric counter part or add the missing symmetric peak.

- peak projection

Calls the PKPROJ commands which "project" the 2D peak table and produce a corresponding 1D peak table.

- SUMREC all peaks

Apply the very simple integration scheme which consists in summing all points over a defined rectangle. This is done by calling the pksumrec macro, which is built over the SUMREC command.

- Integ

Performs a numeric integration of the data-set by computing masks around each peak in the peak table, and integrating over these masks. Equivalent to the `INTEG %%` command.

- Show Amoeba

Display the masks used by the last INTEG command. Available only in 2D. Equivalent to the `SHOW AMOEBA` command.

- ShowPeaks

Display graphically the peaks on the current display. Equivalent to the `SHOWPEAKS` command.

- PlotPeaks

Equivalent to ShowPeaks but on a plot file. Equivalent to the `PLOTPEAKS` command

- Linefit

Calls the generic line fitter. You are prompted for the line-shape to fit (Lorentz or Gauss). Equivalent to the `LINEFIT` command.

- Show linefit

Equivalent to the SHOW LINEFIT command. Display the content of the current peak table as a simulated spectrum. Can be used after LINEFIT, but also at any stage.

- Show_fit

Graphically displays the content of the peak table (as obtained for instance, from the last line fitting). Equivalent to the `show_fit` macro.

- Residue

Display the residue of the last line-fitting. Data can be restored with the `GET DATA` command.

- PkList

Lists the content of the internal peak-table. Equivalent to the `PKLIST %%` command.

- PkRead

Reads the content of the peak table on a text file previously stored with PkWrite. Equivalent to the `PKREAD` command.

- PkWrite

Writes the content of the peak table on a text file. Equivalent to the `PKWRITE` command.

Unix Menu

This button holds some facilities for interacting with the UNIX Operating System. All the buttons are implemented through the generic `SH` command. All entries have equivalent macros or commands available in text mode.

- pwd - cd... - more... - ls -l

Realise the Unix counterparts.

- Shell

Opens an XTerm with the current client and server.

- vi...

Opens in `vi` any text file in the current directory.

- vi macro/...

Opens in `vi` any text file in the global macro directory (/usr/local/gifa/macro). Macros in this directory are available to all the Gifa users. Equivalent to the `vim` macro.

- vi ~/macro/...

Opens in `vi` any text file in the personal macro directory ($HOME/macro). Macros in this directory are available to you, wherever the directory you are in. Equivalent to the `vip` macro.

OPERATION PRINCIPLE

Processing NMR data-set, is just issuing a series of correct commands along with correct parameters. You will find starting from here a list of commands, by topics. A list of commands by alphabetic order can be found on an other part of the manual.
Commands are presented here ordered by functionality, and oriented toward the command level, in contrast with the previous chapter oriented toward the user interface. Extending the user interface can be simply done by learning and using these commands, and the macro language.
As you have seen if you have been through the primer, Gifa is an interactive program : it waits for commands from the user. Some commands have parameters some don't; some commands may even have a variable number of parameters depending on some context value (it is a so-called context-dependent grammar).

Different kind of commands

There are two kinds of commands in Gifa : regular commands which actually execute some action (such as FT for Fourier transform), the others are commands which may execute an action but will also change the value of internal parameters of the program (such as LB for line broadening). Such commands will be called contexts.
For instance HELP is a regular command, but DISP1D is a context which handles the parameter describing the state of the graphic 1D window. A good example of this distinction is given by the context LB which defines the default value used for exponential broadening, as compared to the related EM command which actually apply this exponential broadening to the current data-set.
Most of the behaviour of the program depends on these internal parameters (contexts). Another example of a context is DIM which describes whether we are working with 1D 2D or 3D data-sets .
For instance, type :

```
Gifa> DIM 1 ; switches to 1D NMR
Gifa> size ; lists basic parameters
Gifa> DIM 2 ; switches to 2D NMR
Gifa> size ; lists basic parameters
```

(characters following the semicolon are comments)
The effect of the command size (which lists the basic parameters of the current data-set) depends on the state of the context DIM.
Most contexts have associated Gifa variables which permits to evaluate its value during macro execution. See the chapter on variables for details.
Commands can be issued alone, in which case, the command will prompt you for all the values it needs, proposing default ones. Default values may be kept by hitting the `<enter>` key, or may be changed by typing new ones. You can also type the parameters on the same line than the command; the effect is then immediate. When using in-line entry, the different item will be separated by blanks.
Several commands can even be typed on a single line, separated with a blank. For instance to get back to 2D display mode, you could either type :

```
Gifa> DIM 2
Gifa> size
```

or, on a single line :

```
Gifa> DIM 2 size
```

The effect would be the same. The only difference is that the graphic is only refreshed at the end of the command line; this permits to link together related commands, without slowing down the process by useless display (irrelevant in the present example).

Entering spectral parameter

Most commands and macro prompt for parameters. There are general rules for parameter entering which I will try to describe here.

- Some commands prompt for trivial parameters : file name (`READ`), integer number (`DIM` with parameter which can be 1, 2 or 3), etc.. Little to say about these.
- Some commands prompt for spectral coordinates. Coordinates are always prompted as `INDEX` (this could be easily changed in the source, to prompt in the current `UNIT`), and can be entered in any unit : integer values (terminated or not with a i) for indexes; in Hertz by terminating with a h; in ppm with the p suffix; and finally in seconds with the s suffix. e.g.

```
zoom 1 10 10 200 300
zoom 1 10i 10i 200i 300i
zoom 1 8.3p 8.3p 7.5p 6.5p
zoom 1 6000h 6000h 4500h 4000h
```

or even mixed :

```
zoom 1 10 10i 7.5p 4000h
```

actually might defined the same zoom window (values are given as an example)

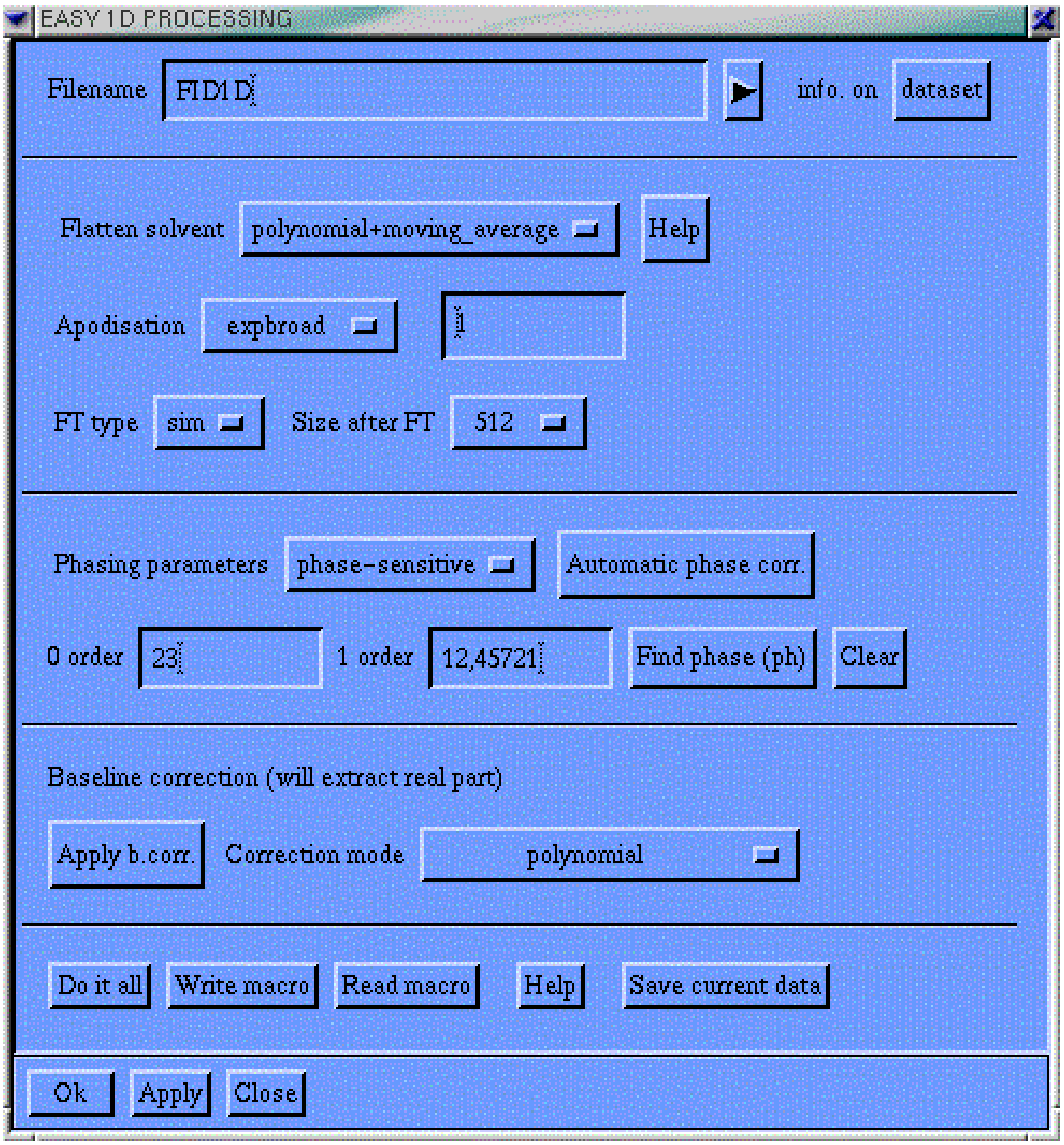
- Some commands prompt for a direction on the current data-set (for 2D and 3D), in which case, axes are called : F1, F2, (F3 if in 3D), sometime combinations are meaningful : F12, (F13, F23, F123). In 2D, F2 is the classical dimension (associated to t2) and F1 is the non classical (t2). In 3D, F3 is the classical dimension, F1 is the slowest non-classical and F2 is the intermediate one.
- Some commands ask for a parameter per spectral axis, in which case, F1 is always prompted first, then F2 (and finally F3).
- Some commands ask for a list of parameters, and the list has no predefined length : `BCORR 1` (which ask for coordinates), `FORMBOX` which asks for field definitions, etc.. In which case, the list has to be terminated by some character. It will be 0 whenever integer values or coordinates are awaited, and it will be a star "*" whenever strings are awaited.
- Some commands prompt for dimension (CX, CY). All dimensions are in centimetres.

General set-up

The standard way of working on an NMR spectra with Gifa is to hold everything in memory. This is in contrast with most NMR programs that process data on disk files, and permitted by a clever memory management.
So, to process a data-set with Gifa, you generally load it in memory, do most of your processing, plot it, and optionally store the processed data on a file for later processing. This permits a very fast processing on small every-day data-sets. When a larger data-set necessitates to work on a file, then a set of specialised commands permits to use all the regular commands on file.
Gifa presents several buffers to store the data. Three working buffers are available for respectively 1D, 2D and 3D. These 3 buffers are independent for regular processing. The buffer on which you are working depends on the value of the context DIM which takes the value 1, 2 or 3.
All the commands refers to the current buffer (as selected by DIM). Depending on the value of DIM, some commands may ask for a varying number of parameters (1 per dimensions) others may ask for direction, in which case the direction is selected with the syntax Fx. In 2D : F2 for the acquisition dimension, F1 for the other and F12 for both. In 3D : F3 for the acquisition dimension, F1 for the slowest dimension, F2 for the intermediate dimension, and F12, F13, F23 and F123 for combinations. When a command requires a parameter for each dimension, F1 parameters will be entered first, then F2 and finally F3 (if in 3D), this rule is general, with the exception of graphical commands which will ask for X and then Y parameters.

BASIC (1D) PROCESSING

easy1d



EASY 1D PROCESSING

Filename: FID1D
info. on dataset

Flatten solvent: polynomial+moving_average | Help

Apodisation: expbroad | 1

FT type: sim | Size after FT: 512

Phasing parameters: phase-sensitive | Automatic phase corr.

0 order: 23 | 1 order: 12,45721 | Find phase (ph) | Clear

Baseline correction (will extract real part)

Apply b.corr. | Correction mode: polynomial

Do it all | Write macro | Read macro | Help | Save current data

Ok | Apply | Close

This macro has been designed to help the user in processing every day 1D data-sets. It consists simply in filling each field of the formbox.

- Filename is the name of the raw data-set which will be loaded before processing.
- A Bruker digital filter correction is applied when data come from a DMX spectrometer (in the Bruker version).
- Flatten solvent let you choose the way of erasing, or not, the solvent. The solvent being located at the center of the spectral width.
- All apodisations are fully available.
- As well as the sizes and the types of the Fourier transform.

- The phase correction and the base-line correction can be also chosen.
- Use 'Find phase' for interactive phasing, or choose 'Automatic phasing'.
- Finally a set of action buttons permits to realize all or some of these operations, additionally, the processing set-up can be stored as a macro file, which when executed latter on, realizes the very same processing. This macro file can also be read back and used to fill the fields of a new form. You can also save your current data at any time of your transform operations.

Loading and Saving data-sets : READ, WRITE, READx, WRITEx, ZEROING

You can load an NMR data-set by typing the READ command. It will load the data-set in the working memory.

In Gifa there is no distinction between time-domain (FIDs) and frequency domain. This is true when processing data-sets (so all the comands are available on all the kind of data-sets), and is also true when storing files. So files contain time or frequency domain data-set, without any distinction.

Several file format are available directly from within the program (plus the utilities permitting to translate from other file formats). The following format are available :

- `READ` or `READC` (same command) for the standard Gifa cached format, the file is stored in a submatrix format, the parameters are in text format in the header part of the file (can be viewed with more);
- `READH` is for the ft-nmr format;
- `READL` is for NMR1/NMR2 format;
- `READV` is for Varian format. The corresponding write commands are `WRITE` (or `WRITEC`) `WRITEH` and `WRITEL` (no `WRITEV` available so far).

Several other file formats are available :

- `READM` and `WRITEM` reads and writes text files, formatted as one line per row for a 2D data-set, and a single line for 1D (not available for 3D data-sets). This format is compatible with the -ascii format of the MATLAB© program. Note however that no parameters are stored along with the data, and that the text file might have very long line that will overflow most text editors.

- `READT` and `WRITET` handle data file in generic text format; on entry per line, with a set of parameters; this permits to import and export data from Gifa to any other program.

- `READS` and `WRITES` are special file format stored in compacted text format; this format is totally independent from the machine used, the file thus stored can be read with the Gifa program running on any machine. This format is in text format and can be safely sent on E-Mail (however you should take care not to send too large files, and eventually cut your large files in smaller pieces (size ² 100kbyte)).

- Finally a `READZ` `WRITEZ` format is available, this format make use of Linear Predictive Coding to compress the data before storing (J.Magn.Reson. 1991). The `WRITEZ` command uses the value of the `ORDER` context as the length of the Linear Predictive Polynomial (see chapter on Linear Prediction). The default value of 10 seems to be an optimum for most NMR data-sets. The compression is performed with no loss of information, with a compression ratio typically in the 50% - 60%. To be used only on time domain data-sets.

Another possibility has been set-up to permits data-set compression. The `ZEROING` command will set to zero all points below a given threshold. Files thus processed will compress MUCH better than regular files. For instance, on a standard TOCSY on *E.Coli* thioredoxin 3mM, using gzip

compressed	**uncompr**	**ratio**	
1945574	2101248	7.4%	standard file
870750	2101248	58.5%	after zeroing $noise ; barely visible
149825	2101248	92.8%	after ZEROING (3*$noise),more drastic, but all peaks are still there

Apodisation : EM, LB, GM, GB, SIN, SQSIN, TM

A comprehensive set of apodisation function is available :

- `EM` is for exponential broadening. The parameter is the broadening applied in Hz. Negative values are possible and are for resolution enhancement (associated with GM). The value used is given by the value in the context `LB`. In 2D and 3D, will apply a different exponential apodisation on axis and will prompt you for a width for each axis consecutively. If you do not wish to modify on a given axis, enter a null value.

- `GM` is for Gaussian broadening. The parameter is the broadening applied in Hz. The value used is given by the value in the context GB.
  `LB` and `GB` are also used in Maximum Entropy processing.

- `SIN` is for a shifted sine-bell. The parameter is the position of the maximum of sine-bell, varying form 0 (pure cosine) to 0.5 (pure sine). The parameter of `SIN` is not kept in a context.

- `SQSIN` is equivalent to SIN but applies a SQuared SINe-bell.

- `TM` is for trapezoidal windowing, and it uses two parameters which are the coordinates (in points) of the 2 points T1 and T2. The window then goes from 0.0 value at the first point of the data set to 1.0 at T1 and from the 1.0 value at point T2 to 0.0 at the last point plus one of the data set.

In 1D, you can use the sequence :

```
Gifa> ONE SIN .3 ; or any other apodisation
```

to visualise the effect of a given filter.

Zero-filling : CHSIZE

Truncation and zero-filling can be applied by the `CHSIZE` command which changes the size(s) of the data-set. You can then truncate a FID or append zeros and the end. `CHSIZE` can be used on any data-set, not only on FIDs, but the `EXTRACT` is preferable for spectra. The zero filling capabilities in the Graphic User interface uses the `CHSIZE` command associated to the power2() function.

basic Fourier transform : ft_sim ft_seq

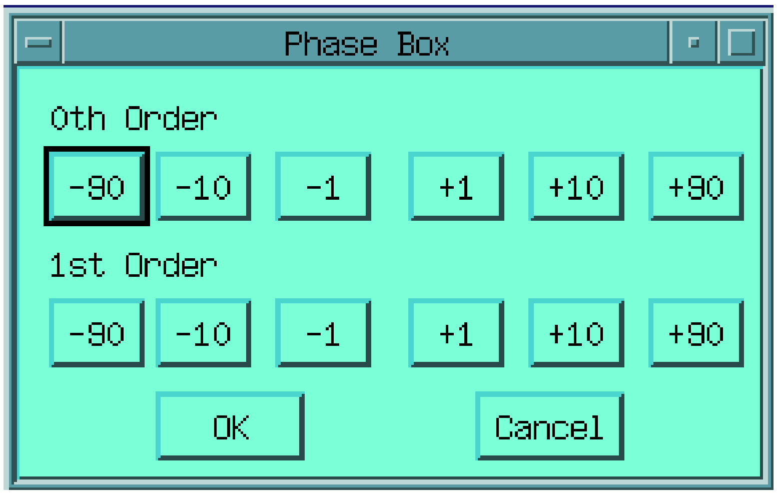
These commands are for the basic Fourier transform step. They realizes the Fourier transform in the acquisition dimension (F2 in 2D, F3 in 3D). `ft_sim` is for complex acquisition (simultaneous sampling of complex and imaginary points); `ft_seq` is for interlaced acquisition of real and imaginary points (1D TPPI).

nD Fourier transform : ft_sh ft_tppi ft_sh_tppi ft_phase_modu ft_n+p

In 2D and 3D the Fourier transform along the non classical axis is performed with another set of macros. The number of way you can acquire the data along the incremental axis of a 2D is much larger than what can be done in the acquisition axis. These macro implements the FT for the more common acquisition mode.

- `ft_sh` performs the Fourier transform for datasets acquired in States-Haberkorn mode
- `ft_tppi` performs the Fourier transform for datasets acquired in Time Proportional Phase Increment
- `ft_sh_tppi` performs the Fourier transform for datasets acquired in the mixture of the 2 previous modes
- `ft_phase_modu` performs the Fourier transform for datasets acquired in phase modulation (J-Modulated for instance)
- `ft_n+p` performs the Fourier transform for datasets acquired with Pulsed Field Gradients in echo/antiecho mode.

Phasing : PHASE, PH, HPHASE, apsl (automatic phasing)



Phasing of the data can be applied with PHASE a b. The 2 parameters a and b, are respectively the 0th order (frequency independent) and 1st order (frequency linearly dependent) phase corrections. In 2D and 3D, axis on which phase correction should be applied is also entered. The pivot for the first order correction is always the centre point of the spectrum. PH is an interactive mode for phasing 1D data-sets.

you can choose and move around your pivot (the double line) by clicking on the spectrum with the second button of the mouse, and you can add phase corrections using the Dialogue box. You can zoom in and out, selecting the zoom box with the first button. Clicking "OK" will finish the PH mode, leave the spectrum phased and load the PHASE default values with the one you just chose, clicking "CANCEL" will exit the PH mode as if nothing had happen. HPHASE permits to phase real data-sets, with the same syntax as PHASE.

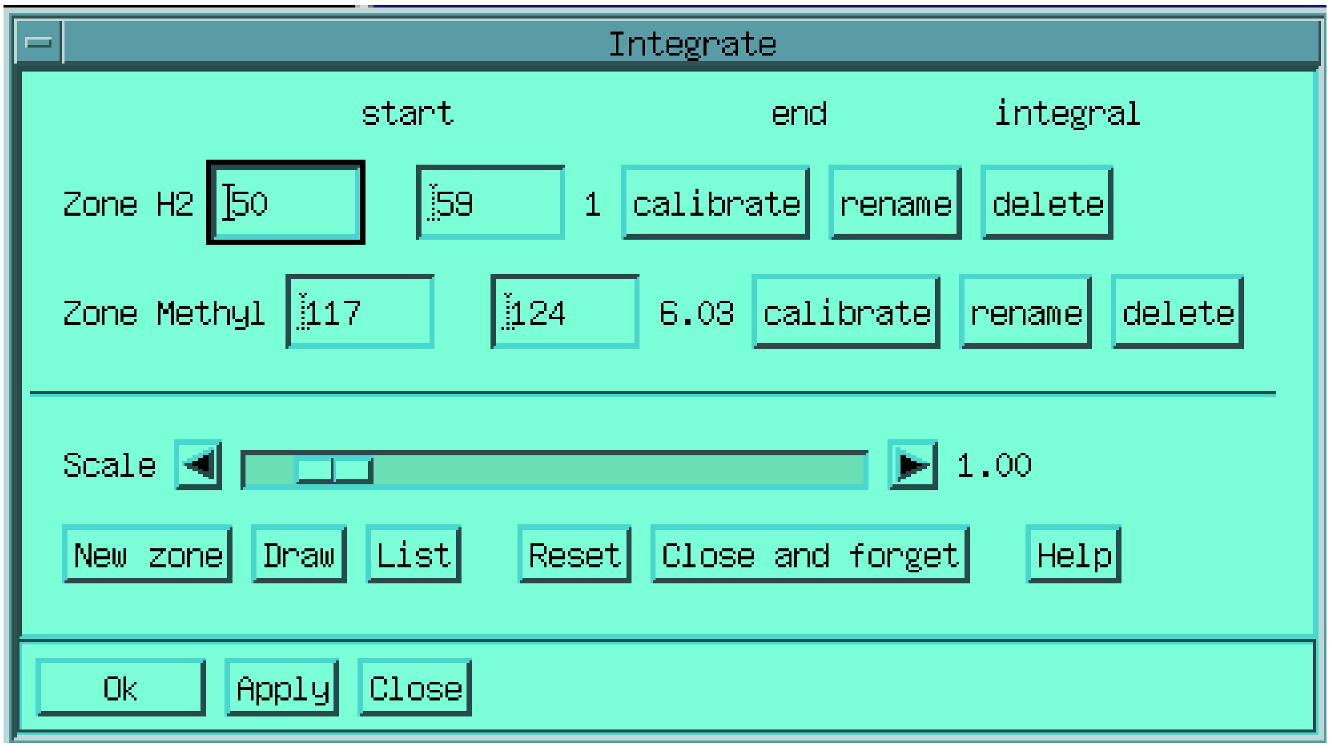
`HPHASE` performs a Hilbert transform in order to create the missing imaginary part, it thus permits to phase a real spectrum by creating the imaginary part on fly.

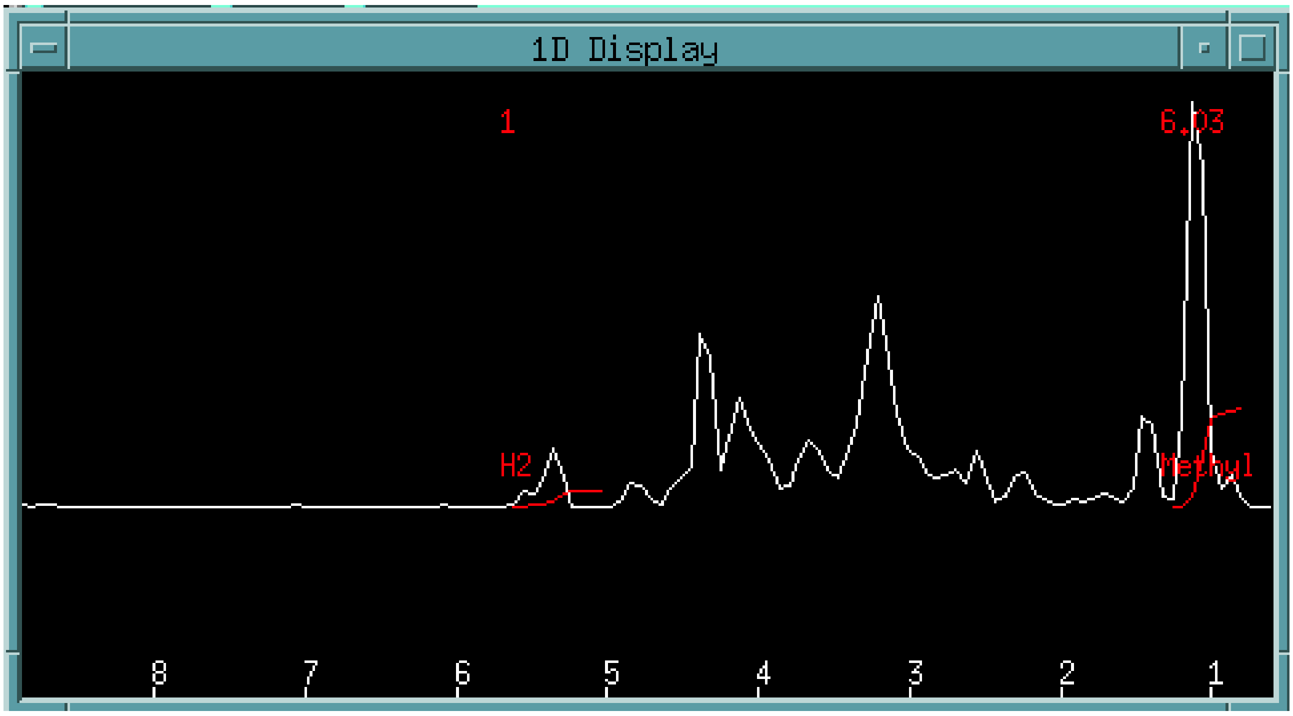
The sequence `IFTBIS FT` will create a complex spectrum from a real one (with half the resolution), thus permitting to experiment phase parameters with the PH command. These phase parameters can then be used on the corresponding original real spectrum.

An automatic phasing method have been made available in Gifa lately : it is the APSL method (by A.Heuer, *J.Magn.Reson*. **91**, p241-253 (1991)). This method works by using the symmetry of the phased line. A macro have been written which implements this method, it is called `apsl`, and works in 1D.

Integration

Start the 1D graphic integration module. Here is an example of an integration, with 2 zones defined. And you get on screen :





From there, you can create and delete integration zones; calibrate one zone to a given value and all other zones will adapt; or even create a listing :
Note that the base line should be corrected before hand. Accurate integration values can also be obtained when using the Linefitter.
adapting to your own set-up

The macros present above are intended to be adapted to your own set-up and spectrometer. The way the complex numbers are stored in the FID depends on the spectrometer manufacturer, so these macro should be adapted so that the spectra show correctly after using them. They are based on elementary commands presented below. In the standard distribution, the files are pre-set for usage with Bruker spectrometers. A series of adapted macros are available for Varian users in the directory: `/usr/local/gifa/macro/varian`. Have a look to the README file in there.

You can easily customise your set-up to use the Varian macros by default by adding the varian directory to your GifaPath. This is done by adding the following line :

```
SETPATH ('/usr/local/gifa/macro/varian'; $GIFAPATH)
```

at the end of the set-up file: `/usr/local/gifa/macro/startup.g`
This should be done for each new version of Gifa you download. (See customising the interface for details)

Detailed Fourier transform : REVF, FT, IFT, RFT, IRFT, FTBIS, IFTBIS, INVF, REVERSE; Hilbert transform

These commands details the elementary steps of the basic Fourier transform.
The elementary Fourier transforms available are :

- `FT IFT` : complex to complex FT and its inverse
- `RFT IRFT` : real to complex FT and its inverse
- `FTBIS IFTBIS` : complex to real FT and its inverse

The complete set of Fourier transform can also be summarised as follow (C stands for Complex and R for real) :

```
        FIDs            Spectra
C       ~FT->   C
C       <-IFT~  C
R       ~RFT->  C
R       <-IRFT~ C
C       ~FTBIS->        R
C       <-IFTBIS~       R
R       Does not exist  R
```

The Hilbert transform is simply realised by :

- `IFTBIS FT ; generate a complex data set from a real`
- `IFTBIS PHASE 90 0 FTBIS ; generate the missing imaginary part`
- `IFT FTBIS ; in-place zero filling using Hilbert relations`

Depending on the spectrometer the data you get should usually be processed with FT (complex FT) or RFT (real FT) and eventually pre-processed with REVF. REVF actually inverses every 2 points over 4. This has the effect to reduce the time-proportional format used for the seq mode on BRUKER spectrometers (on real data-sets).
On complex data-set it has the effect to put the zero-frequency on the borders of the spectrum (after the FT step!).
INVF is related to REVF, it inverse every other point in the data set, thus taking the conjugated value on complex data-sets. Because of this, the sequences : INVF FT and FT REVERSE are equivalent. On hypercomplex data (2D) INVF F12 will take the hyperconjugated.
REVERSE simply returns the current spectra left to right.

Data-type : ITYPE

1D Data-set are either real or complex. On multidimensional data-set (2D or 3D), each direction may be either real or complex. This the so-called hypercomplex data-type.
The type of the data-set (real or complex) is described by the context `ITYPE`.

For 1D, ITYPE is 0 for real data and 1 for complex data.

For 2D, ITYPE can takes 4 different values :

- 0 means real;
- 1 means complex in the F2 direction
- 2 means complex in the F1 direction (I know, this is a bit odd but has to make sense in 1D as well as in 2D)
- 3 means complex in both directions (so-called Hypercomplex data type).

In 3D

- 1 means complex in F3
- 2 complex in F2
- 4 complex in F1
- and the corresponding sums depending on the hypercomplex state of the data-set. For instance
- 7 means that the data-set is complex in all axes.

Certain commands require a specific ITYPE value. For instance FT is available only on complex data sets. An error message will be given if an FT is tried on a real data-set. Note that if the data is complex, the real part is held in odd points of the buffer, the imaginary part is held in the even points. ITYPE is usually handled automatically by the program, so the user does not need to worry about it. You may however have to change it in certain cases, typically when loading the data-set the first time, when "playing around" with the data-set, or when a "bug" happens in the program (highly unlikely......!?)

ADD, ADDH, ADDDATA, MULT, MULTDATA

Two data-sets (1D, 2D or 3D) can be added together with the ADD command which prompts you for a file-name, then adds the current data-set along with the content of the file "file-name" in standard format, the result being left in memory.

It is also possible to add a file in FT-NMR format with the ADDH command.

Finally it is also possible to add the current buffer with the data held into the DATA buffer with the ADDDATA command (single word).

In all cases, you may want to pre-scale the current data-set with the command `MULT` which allows one to multiply the current data-set by a given scalar.

The command `MULTDATA`, on the other hand, multiplies point by point the content of the current buffer with the content of the `DATA` buffer. This permits to realise convolution product. When applied on complex (respectively hypercomplex) data-sets, a complex (respectively hypercomplex) product is realised. (See Several Buffers) for more multi buffer commands

Post processing : REAL, SWA, USWA, ABS, MODULUS, PLUS, MINUS, ZEROING, SMOOTH, MEDIAN

These commands are meant for post-processing of spectra after Fourier transformation :

`REAL` will remove the imaginary part of a complex data-set, thus halving of the size of the file of a phased spectrum.

`USWA` will separate the real and imaginary part of a complex data-set, they will be displayed on each side of the data-set, changing its `ITYPE` from complex to real, thus permitting to examine both part at the same time.

`SWA` performs the inverse of `USWA` by taking each side of a real data-set as real and imaginary parts of a complex data-set. Both `SWA` and `USWA` will only work on data with a size equal to a power of two. If it is not the case, you will have to add zeros up to the next power of 2, apply the command, and then reduce the size to the previous value.

`ABS` will compute the absolute value of the current real data set.

`MODULUS` will compute the modulus of the current complex data-set and put the result in a new real data-set. In 2D the action taken will depend on the value of `ITYPE` :

- `ITYPE=3`, the hypercomplex modulus = $\sqrt{RR^2 + II^2 + RI^2 + IR^2}$ will be computed
- `ITYPE=1`, the complex modulus = $\sqrt{R^2 + I^2}$ will be computed along F2
- `ITYPE=2` is not handle and the data should be modified with FLOP.

In 3D, the modulus will be computed only for fully hypercomplex data-sets (`ITYPE = 7`).

`PLUS` and `MINUS` will put to zero all the negative points (the positive for `MINUS`), thus leaving a purely positive (negative) data-set.

`ZEROING` will set to zero all points below a given threshold (very useful for compacting processed data-file see above at `WRITE`).

`SMOOTH` and `MEDIAN` are after-processing filters. `SMOOTH` realises a moving-average smoothing of the data set on a window of variable length, whereas `MEDIAN` will perform a median filter on the data-set, by taking the ith smaller value of the moving window. Both `MEDIAN` and `SMOOTH` will change the data-set size by the number of point of the moving window.

EVALN, ADDBASE, NOISE, SHIFT

Permits to compute the noise level and the systematic offset of the current data-set within a given window. Computed noise level will be put into the context `NOISE`, the systematic offset will be in `SHIFT`.
`ADDBASE` will remove a given systematic offset on the data-set. The command prompts you with the last value computed by `EVALN`.
A macro: evaln.g implements a graphical interface to `EVALN`, permitting to compute noise in a graphically given window.

DSA

Implements the Digital Shifted Acquisition method which permits reduction of the water signal after acquisition (if the water signal is at zero-frequency). This command will actually add the actual data with itself, after a shift and multiplication. Values of -2 for the shift and -1.0 for the multiplication factor will remove the water signal at zero frequency on a BRUKER data-set. You can notice that there are also several other ways of removing the water by the flatten solvent correction methods.

HANDLING OF 2D AND 3D DATA-SETS

Introduction to 2D and 3D processing

Processing of 2D and 3D data-sets is similar to 1D data-sets in many respects. The processing steps are mostly equivalent : reading the file, windowing, pre-processing and zero-filling, Fourier transformation, Post-Processing (phasing, smoothing, REAL etc...) and writing output file. This is due to the fact that the whole data-set is merely held into central memory.
This design is optimum whenever the data-set is small enough to be kept in memory without even using the disk (up to 2 Mega (2D : 1Kx2K or 3D : 128x128x128) points on a typical system). The main drawback is that there is a definitive upper-limit for the size of the data-set. This limit depends on your system, but is typically 4 Mega (2D : 2Kx2K or 3D : 128x128x256) on most small to middle work-stations, and 16 Mega (2D : 4Kx4K or 3D : 256x256x256) on larger machines. This setting can easily be modified by recompiling the program. If you need to work on a larger data-set, you will have to resort to the cache memory system.

The working buffer and the DIM command.

The state of the program is described by the `DIM` context which holds either 1, 2 or 3 (standing for 1D 2D and 3D). Each mode is associated to a buffer, thus there are 3 buffers, for 1D, 2D and 3D. The unselected buffers remains unchanged during the processing of other buffers. All commands refer to the current working buffer, and most of the commands works on all three modes, however, the commands may change their behaviour depending on DIM. The command DIM permits to change the current working buffer, and can take the values 1, 2 or 3. When the graphic user interface is used, the 1D th 2D and the 3D command are separated, and a error will be issued if you use a 1D command (say) in 2D mode.

Different behaviours

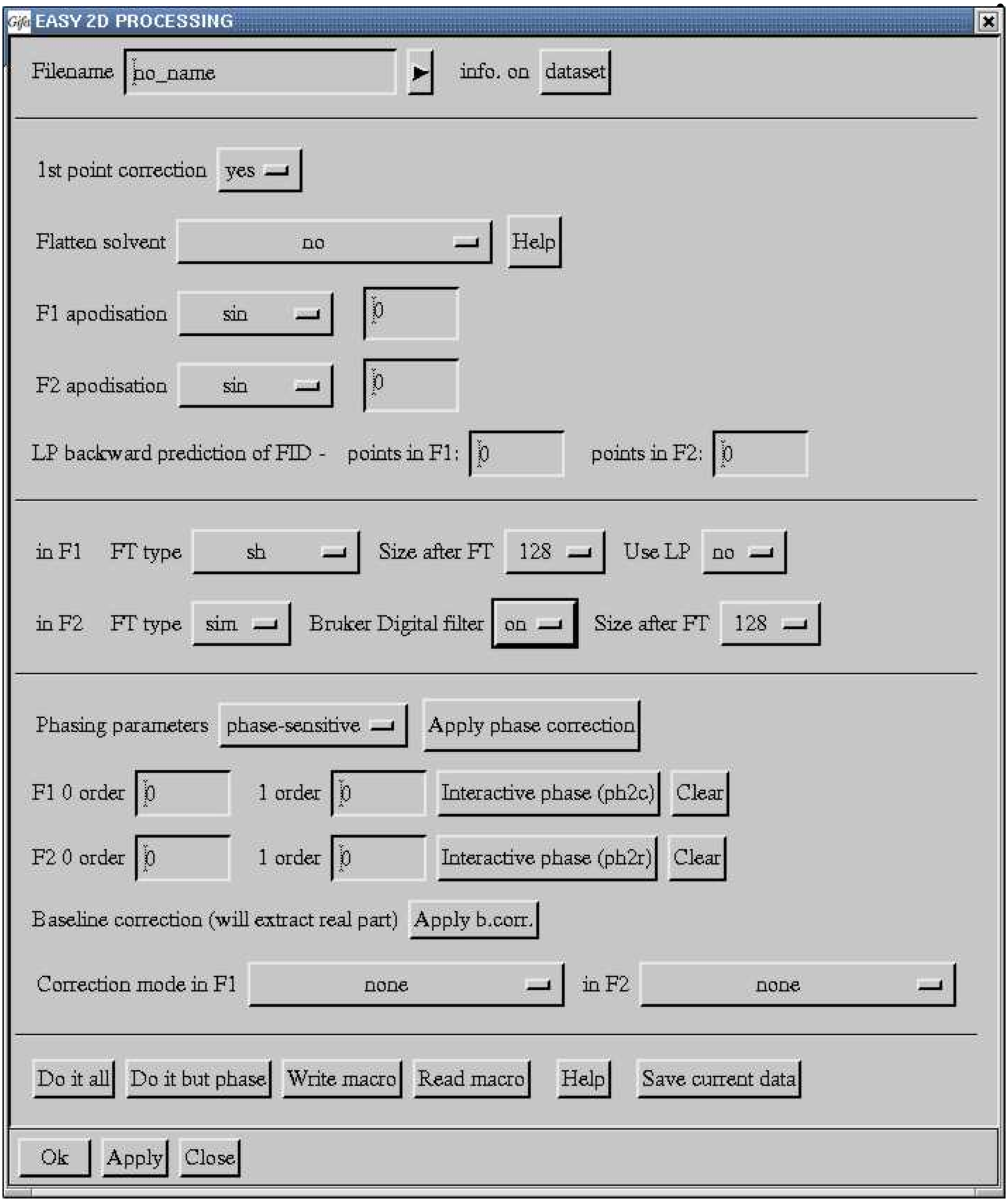
When calling a command from the prompt line, or in macro processing each command will react differently depending on the current DIM chosen. Some commands are completly independent on DIM (such as `READ, WRITE, ZERO, PEAK,` etc..). Some will take one argument in DIM1, two in DIM 2 or three in DIM 3 (`CHSIZE, EM, GM, SPECW, ZOOM`, etc...). In this case, in 2D the arguments are ALWAYS in the order : slow varying dim. (F1) then acquisition dim. (F2) and in 3D, in the order : slower varying dim (F1) intermediate (F2) and acquisition dim (F3).
Finally some commands (such as `FT, SIN, PHASE, REVERSE, BCORR`, etc...) will have an additional argument telling along which axis the command should be applied in which case the axis is either F1 or F2 in 2D and F1, F2 or F3 in 3D, combinations such as F12 or F13 F23 F123 (in 3D) are possible.

Commands more specific to 2D data-sets or 3D data-set

Some command are strictly restricted to 2D or 3D handling or processing. First you should learn how to use the `easy2d / easy3d` macro, and when you are at ease with this processing switch to more specific commands.

easy2d

This macro has been designed to help the user in processing every day 2D data-sets. It consists simply in filling each field of the formbox.



EASY 2D PROCESSING

Filename: no_name — info. on dataset

1st point correction: yes

Flatten solvent: no — Help

F1 apodisation: sin — 0

F2 apodisation: sin — 0

LP backward prediction of FID - points in F1: 0 — points in F2: 0

in F1 — FT type: sh — Size after FT: 128 — Use LP: no

in F2 — FT type: sim — Bruker Digital filter: on — Size after FT: 128

Phasing parameters: phase-sensitive — Apply phase correction

F1 0 order: 0 — 1 order: 0 — Interactive phase (ph2c) — Clear

F2 0 order: 0 — 1 order: 0 — Interactive phase (ph2r) — Clear

Baseline correction (will extract real part) — Apply b.corr.

Correction mode in F1: none — in F2: none

Do it all — Do it but phase — Write macro — Read macro — Help — Save current data

Ok — Apply — Close

Filename is the name of the raw data-set which will be loaded before processing. If you click on the `dataset` button, you will see (in the terminal window) the characteristic of the file currently selected.

- 1st point correction modifies the data-set in order to reduce the 't1-ridges'.

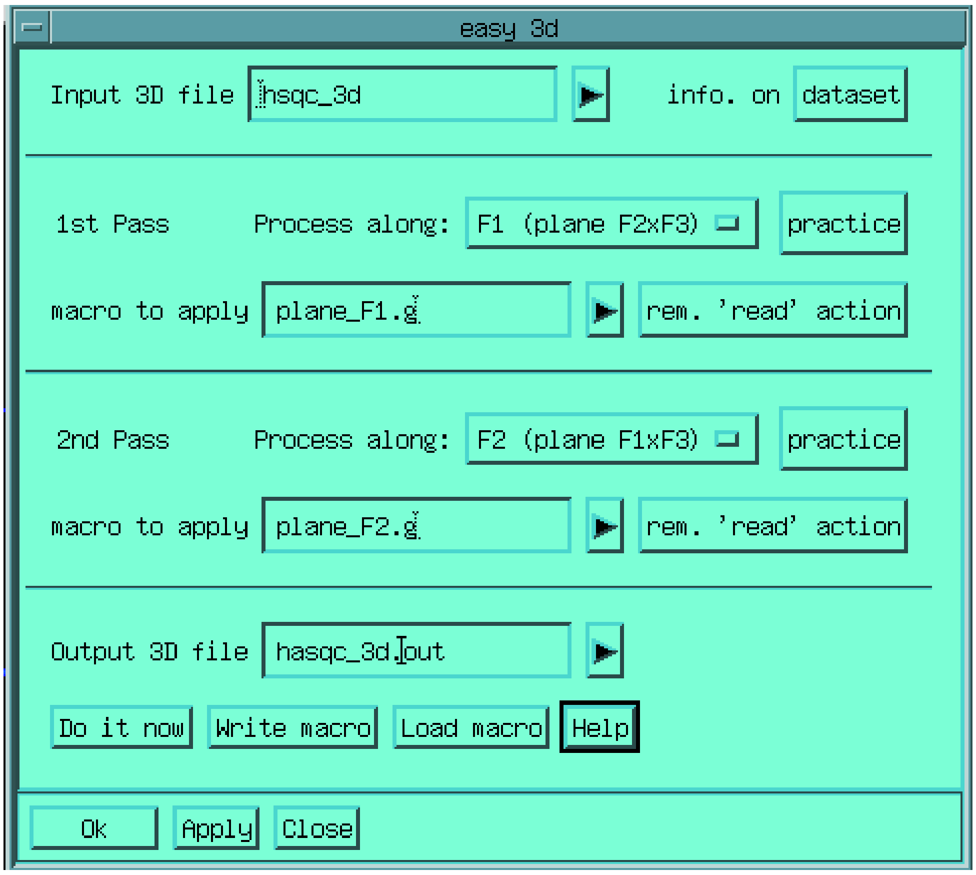
- A Bruker digital filter correction is applied when data come from a DMX spectrometer (in the Bruker version).
- Flatten solvent let you choose the way you will (or not) remove the water or other solvent. The solvent being located at the center of the spectral width.

- All F1 and F2 apodisations are fully available.

- As well as the sizes and the types of the Fourier transform
- The phase corrections and the base-line corrections can be chosen interactively. The applied phases are cumulated in the 4 independent phase parameters displayed on the form.
- Finally a set of action buttons permits to realize all or some of these operations, additionally, the processing set-up can be stored as a macro file, which when executed latter on, realizes the very same processing. This macro file can also be read back and used to fill the fields of a new form, and the current data can be saved on demand.
- The macro will switch by itself to on-file processing if the file is too large to be processed in memory. In which case, you will have to ressort to the additionnal 2D_on_file menu for further interaction with this 2D file.
- Processing will switch automatically to on-file processing if the size of the data-set is too large to be handled in memory. In which case, the `write macro` action will write a on-file processing macro

easy3d

This macro has been designed to help the user in processing every day 3D data-sets. Its use is very different from the `easy2d` macro.


easy 3d

Input 3D file: hsqc_3d
info. on: dataset

1st Pass — Process along: F1 (plane F2xF3)
macro to apply: plane_F1.g

2nd Pass — Process along: F2 (plane F1xF3)
macro to apply: plane_F2.g

Output 3D file: hasqc_3d.out

The principle is the following

- `Input 3D` file is the name of the raw data-set which will be processed
  if you click on the `dataset` button, you will see (in the terminal window) the characteristic of the file currently selected.
- You select the kind of plane you want to process during the pass, then clicking on `practice`, you will get the first plane as 2D, and will be able to find correct processing conditions with the `easy2d` user interface.
- Once set-up, write the macro with the default name (for instance `plane_F1.g` if processing F1 planes), then hit the `rem. 'read' action` button in order to adapt the macro to 3D processing.
- Using the `Do it now` button, will start the processing, using the defined macro for all selected planes of the 3D.

- You can choose to have only on pass processing, by choosing `'none'` as plane type for one of the pass. If you choose to have two passes, then a intermediate file will be created.
- The `write macro` and `Load macro` buttons have the same meaning as in easy2d.

COL and ROW (2D & 3D)

Permits to access directly any row (along F2) or column (along F1) of the data set. It is put into the 1D buffer and is displayed in the 1D window. In 3D, will extract rows and cols from the last selected plane (see `PLANE`).

PROJ (2D & 3D), proj_loc

In 2D will compute the projection of the current data-set along one axis. Axis along which the projection is computed has to be entered, thus PROJ F1, will compute the projection along F1 onto F2. Two algorithms are available : mean value or skyline. Result will be put into 1D buffer.
In 3D, the projection along one axis, onto a plane will be computed and put into the 2D buffer
On the other hand, the macro proj_loc computes the projections of a defined region of the spectrum.

FLIP and FLOP (2D & 3D)

In 2D, permit to go back and forth from `ITYPE=1` to `ITYPE=2` data-sets by changing the way the imaginary part is interleaved, i.e. the imaginary part is exchanged between F1 and F2 axes. For instance the following sequence :

```
Gifa> FT F2 FLIP FT F1
```

will perform the classical complex Fourier Transform (not hypercomplex). These commands are used when processing phase modulated data-sets. The sequence :

```
Gifa> REVF F2 RFT F2 FLIP REVF F1 INVF FT F1 FLOP MODULUS
```

will perform the computation of a phase-modulated data-set acquired on a BRUKER spectrometer in sequential mode.
In 3D, you can exchange the imaginary part of the F3 axis with the F1 or F2 axis.

SYM

Symmetrises the current 2D relative to the main diagonal (COSY-type). Each point is compared to its symmetrical, and is replaced by either the mean value of both location, or the smallest of both location.

TRANSPOSE (2D & 3D)

Transposes the 2D matrix . The sizes of the matrix must be power of two for this command to be used. After transposition, the two dimensions are completely permuted. In 3D, 2 dimensions will be exchanged by the `TRANSPOSE` process.
Transposition is not a natural step when working with Gifa, all the processing can always be performed randomly in any axis.
The transpose process is performed in-place and is very time consuming. On typical systems it is probably faster not to transpose when processing the data set. On very small system with very limited physical memory, it may be faster to use transpose. Try comparing

```
Gifa> FT F2 FT F1 ; normal processing
```

to

```
Gifa> FT F2 TRANSPOSE FT F2 ; transpose during process
```

on your system
Up to now, it seems that `TRANSPOSE` is completely buggy in 3D !

PLANE (3D)

Will select a plane from the 3D data-set, and put it in the 2D buffer. Plane are select by the name of the orthogonal axis : i.e.

```
Gifa> plane F2 index
```

will select the plane holding the F1 and F3 dimension, at coordinates F2=*index*.

VERT (3D)

Will select a line orthogonal to the currently selected plane. You can choose the coordinates by pointing on the 2D display.

DIAG (2D & 3D)

In 2D `DIAG` will permit to extract the main diagonal of the current data-set. In 3D, it will extract one of the three main diagonal plane of the cube (F1=F2, F1=F3, F2=F3). Extracting the main diagonal 1D of the 3D cube can be done by extracting the 1D diagonal of one of the diagonal plane of the cube.

BASELINE CORRECTION : BCORR

BCORR is a comprehensive base-line correction module. Linear, cubic spline or polynomial base-line correction algorithms can be selected. The 2 first modes will use a set of points or "pivot" points to compute the base-line. A given radius is used around each pivot point for averaging the pivot value. Linear mode will then realise a linear regression through the pivots points and remove the linear baseline thus found. If only one point is given, then a horizontal baseline is computed. Spline mode will compute a cubic spline going through the pivot points and remove it from the data set. Spline mode requires at least 3 pivot points to work. BCORR proposes as default values for the index of the pivot points, the last clicked points with the point (the values in the point stack) command; you can thus use the %% syntax.
A third option is available in BCORR, corresponding to polynomial (and related) baseline correction. This last option of the baseline correction is modular. The correction is made in three steps:

- First the signals and the baseline are separated in zones (referred in the following as the first segmentation), this first segmentation is eventually helped by a temporary smoothing of the data,
- These zones are then joined together in several sets of related area (referred in the following as the second segmentation)
- The correction is finally computed.

There are three general parameters :

BLOCBASE : all parameters in point unit are scaled in the ratio of the data set size to this parameter.

BLCITER : the maximum number of iterations for the whole process

BLCW : when the RMS of the correction is lower than BLCW times the RMS of the data, the correction is finished.
There are several commands and parameters to configure the correction :

SMOOTH1 : controls the smoothing of data.

- 0 : no smoothing.
- +1 : moving average of the data set on a window of WINMA points.

- +10 : hysteresis smoothing of the data set with the value `LEVELHYSTE`.

`SEGM1` : you can choose the way the first segmentation is done as follows .

- 0 : without.
- 1 : with a standard deviation algorithm on the data set.
- 2 : with a standard deviation algorithm on the first derivative of the data set.
- 3 : with thresholds on the data set, and on the first and second derivatives.
- 4 : with a dynamic clusters algorithm.
- +10 : with a morphological filtering after the segmentation.

The two parameters used by the standard deviation algorithm are `BLCU` and `BLCV`. You should only use `BLCV`, for example if you increase `BLCV` you reduce the sensibility of detection in order to correct a dispersive line shape.
The threshold option just remain for historical means, the four thresholds are `SDS, SDB, SCB, SCS`.
The dynamic clusters algorithm is controlled by four commands :

`DCALGO` : select the data on which the algorithm operates.

- +1 : the algorithm runs on the data set.
- +10 : the algorithm runs on the first derivative of the data set.
- +100 : the algorithm runs on the second derivative of the data set.

`DCDISTANCE` :

- 0 : Norm 1.
- 1 : Euclidean distance.

`DCITER` : the maximum number of iterations for the dynamic clusters algorithm.

`DCFACTOR` : used in a logarithmic scaling of the data set.

Then you can add a morphological filtering either on the baseline selection or on the signal selection by choosing a number of points with MORPHOB and MORPHOS.

`SEGM2` : this feature is only useful with a polynomial approximation.

- 0 : without.
- 1 : interactive.
- 2 : automatic.

When you choose an interactive second segmentation, you have to choose one or several areas with the `WINDOW` command to allow the program to cut the correction in these areas if needed.
The automatic segmentation uses a window, `WINSEGM2`, and a threshold, `LEVELSEGM2`.

`APPROX` : the last step is to choose the way the baseline is estimated.

- 0 : with ITERMA2 times a moving average filtering on a window of size `WINMA2`.
- 1 : with a Legendre polynomial approximation of degree `DEGRE`.
- +10 : with a linear interpolation of signal before approximation.
- +100 : with an 'elastic effect' that is a rude way to prevent from burying the weak lines.

There are four special commands that may help you with all these options :

`BCORRP0` : restores the initial configuration with a polynomial approximation.
`BCORRP1` : enable a configuration with a dynamic clusters segmentation and a moving average approximation.
`BCORRP?` : lists the current configuration.
`BCORRP` : a step by step command to choose a set up.

SPECTRAL PARAMETERS

SPECW, OFFSET, UNIT, UNIT_Y FREQ

These contexts describe the spectral widths (`SPECW`) of the spectrum and offset (`OFFSET`) of the right-most point of the current data-set, thus creating a frequency reference for the data-set. Values are in Hz. Frequencies are used by `EM`, `GM`, and changed by `EXTRACT` (but not `CHSIZE`, be careful.). The calib macro permits to set the offset in an interactive manner. When no information is available on the current data-set the `OFFSET` is set to 0 and the spectral widths to 2000*Pi.
The context `FREQ` holds the basic frequency of the spectrometer (in MHz). It is used to compute ppm from Hz.
The context `UNIT` will tell other commands (`AXIS`, `POINT`, `PKLIST`, etc...) to choose the unit used. `UNIT` can take the values `INDEX` (number of channel) `HERTZ` (based on `SPECW` and `OFFSET`), `PPM` (`HERTZ` divided by `FREQ`), `SECOND`(based on `SPECW`), `DAMPING` (based on `DMIN` and `DMAX`), or `TABULATED` (based on the `TAB` buffer). All other values are invalid. UNIT_Y is equivalent to UNIT but used only for the vertical axis (F1) of 2D.

size, list

These two macros permits examination of the current state of the data-set. `size` is a simple one-line text. `list` is a comprehensive output.

EXTRACT

permits to extract a given part of a spectrum and thus becoming the new data-set. `EXTRACT` is used as `ZOOM` but is obviously not reversible.

DISPLAY AND GRAPHIC INTERACTION

Display is fully optional in Gifa, when the program starts it detect whether it is connected to an X-window server or not. If it is the case, the standard startup macro installs the menu-bar and opens several default spectral windows. Again these windows can be close at will, or reopened at any time.

DISP1D, DISP2D

When `DISP1D` is one, a 1D graphic window call « 1D Spectrum » is displayed on screen, 1D buffer will be displayed in this window . 2D will be displayed as density colour maps in a square window call « 2D window » when `DISP2D` is 1. In 3D mode, planes extracted from the 3D data-sets will be displayed as 2D. Setting these contexts to 0 actually closes the associated window.

The size of the created windows with the `DISP2D` command, is hard-wired and cannot be modified.
The display is refreshed at only the end of each command line; you can thus avoid useless display of intermediate computation by putting all the related commands on one line.
On VWS window manager, the graphics may sometimes be surrounded by a yellow border (if the sizes are different from a power of two).
2D are displayed in density mode. The density mode consists of a colour coding of the value of the points. 64 colours are used, distributed with a constant interval on positive and negative values. Values around zero are coded in black.

SCALE, ITYPE, ABSMAX, SIGN, VHEIGHT, CLEAR

These contexts characterise the state of the display and the plotting.
The display is computed at the end of the command line. Some point may be skipped when displaying large spectra (typically greater than 4k in 1D, and larger than 512x512 in 2D) but not for plotting. The vertical size of the display is defined by the `SCALE` context. The display depends also on the ITYPE value; imaginary points are not displayed.
The scale is computed such that for `SCALE 1`, the larger point of the spectrum is full-screen. In 2D, the lower level displayed will 1/32 the higher level displayed. The value of this larger point is held in the `ABSMAX` context. `ABSMAX` is recomputed at display time whenever the data actually changed, however it is not recomputed when it is not needed and you can force the computation of `ABSMAX` by putting its value to 0. The scale being relative, `ABSMAX` can be modified to compute absolute display and plot by forcing its value to any pre-defined value. This value will not be overridden as long as the data are not actually changed.
To make this long story short, one can say that the point with the value `ABSMAX` / `SCALE` will be displayed full screen.
Absolute display (to compare spectra, or to set the first level relative to the noise) can be obtained by forcing `ABSMAX`. See the FAQ at the end of the manual for more information and examples.
`SIGN` determined, in 2D or 3D whether only positive points, only negative points or both will displayed.
`VHEIGHT` is the level to which the zero level will be plotted in 1D display. Unit is in %, 0 will draw at the bottom of the screen/page, 1 at the top. Standard value is 0.3 (30%).
`CLEAR` context determines if each display will be drawn on the top of the previous one (0 mode) or if the window will be cleared before drawing (1 mode - default mode).

CDISP2D, LEVEL, LOGA, CCOLOR

A second display mode is available in 2D which is a contour plot mode that is activated with the command `CDISP2D`. The size of the `CDISP2D` window when opened is always 15cm x 15cm. `SCALE` and `SIGN` are active in this window as they are in the density window. The number of contour levels is defined by the `LEVEL` context; `LEVEL` contours are displayed in the positive and in the negative part and are equally spaced between 0 and `ABSMAX` / `SCALE` in the default mode of `LOGA` equal to 1. If the context `LOGA` is set a value larger than 1 then each level is at a position equal to the previous level time `LOGA`. For instance if with `LOGA 1` levels are at :
1 2 3 4 5 6 etc...
with `LOGA 1.5` levels will be :

1 1.5 2.25 3.375 5.0625 7.59 etc...
`LOGA 2` corresponds to the BRUKER standard spacing.
When working full spectrum on large data-set a `CDISP2D` can take too long, and you may wish to stop the display, you can always do it by typing a ^C.
Contour plot display are normally in colours, with a colour code equivalent to the `DISP2D` mode, however it is possible to switch to a Black and White mode with the `CCOLOR` context.

AXIS

This command determines whether coordinates will be drawn on the axes of the current display. Coordinates can be selected to be an all axes, on only one direction, or to be absent. The kind of coordinates which is displayed is determined by the `UNIT` command (see previous chapter).

COLOR, SCOLOR, Choice of Colours

Display are of two kinds : vector mode, used by 1D, 2D contour mode, 3D and the `SHOWxxx` commands; or image used by density mode in 2D. In vector mode the colour used is determined by the `COLOR` context which default value is white. The current colour can be chosen separately for each window with the `COLOR` command. Only 8 colours are available with the `COLOR` command, they correspond to pure colours when the standard colour file is used. The context `SCOLOR` determines the colour used by the `SHOW` and `SHOWxxx` commands (see below).
The colour table used by the density mode is built when starting the program. The presence of a file called `.gifacolor` is checked first in the working directory, then in the $HOME directory, then the presence of a file called `gifacolor` is checked in `/usr/local/gifa/com`. If one of these file is found, it is used as a list of colours to be used by the density display. The file has one entry per line, first the choice of colours for the pointer, then for the density mode, starting with the large negative value ending with large positive values. Each entry is of the form HUE - SATURATION - INTENSITY. If no file is found, a default set up is used. You will find on the distribution tape a set of small programs that permits to build such custom colour tables. The standard colour table, as well as a Black & White colour table are given as example.

will generate a psychedelic effect by rotating the colour tables (on VMS/VWS only). Go ahead and try it, just for the fun of it!

ZOOM, ZM

The `ZM` commands opens a control box which permits to zoom in and out the data-set, to move around the zoom window and to rapidly set the `SCALE` value. To set the zoom window click on the data-set with the left and middle button of the mouse, and then click on the `Zoom In` button (or on the display, with the left and right button of the mouse). Other controls in th `ZM` box are very natural.
Some times, when using some interactive commands or macros (`PH, point, rowint`, ...) the controls of the ZM box remains active even though a watch is displayed in the window. Activating the ZM 1 command when the zoom is already on will recompute the small vignette display, as if the `catch spectrum` button had been clicked.

`ZOOM` is a command which permits to define a zoom window on the data-set in a non graphical way. It is perfectly possible to define a zoom window, even if there is no graphic open. Many commands (`LINEFIT`, `PEAK`, etc..) only apply within the current zoom window

The Point stack : MONOPOINT, POINT_PUSH, POINT_POP, POINT_CLEAR, point_dump, point

`MONOPOINT` will permit just one click on the data-set. Gifa will be blocked until the user actually clicks on the graphic screen. The coordinate of the click is stored on the top of a special stack (the *point stack*). This stack is handled with the 4 commands : `POINT_INPUT` `POINT_PUSH`, `POINT_POP`, `POINT_CLEAR`. The content of this stack is used as default values by many commands (`ZOOM, EVALN, BCORR, POINT->PK`, etc...) In macro programming the content of the point stack is examined through the variables `$POINTX[] $POINTY[]` and `$NPOINT`. The macro `point_dump` prints out the state of this stack.
The macro `point` permits to interact with the data, it is based on `MONOPOINT`. With `point`, the point stack is cleared, and all the clicked points are stored into the stack. Point is exited by clicking on the data-set with the right-most button of the mouse.

SHOW

permits to put some information in the graphic window. `SHOW` takes an argument : `CURRENT` will show the current data-set as-is; `FT` will show the FT of it. Other parameters are available, see below or the alphabetic list.

FREEZE

freezes the current graphic window making it inactive, and create a new one equivalent to the previous. This is useful for comparing data.

REF, UNREF, REFMACRO

These command are mostly used when fine tuning the display during macro programming.
`REF` will force a new computing of the display, as if a display command had been issued. This is useful for cleaning the spectrum after a point or whatever command, it can be called from the `ZM` box.
`UNREF` realizes just the inverse, i.e. display will not be refreshed, even if the previous commands did modify the data-set. `UNREF` is useful in macro for fine control on the display. It is active only for the commands that precedes it in the command line / macro ; so it is usually the last command issued.
`REFMACRO` controls whether display will be done at the end of each command line within macro. Default value of 0 means no refreshing during macro execution, which permits much faster execution. If you write interactive macros with graphical display, you should set `REFMACRO` to 1. It is often useful to change `REFMACRO` several time within a macro.

PLOTTING

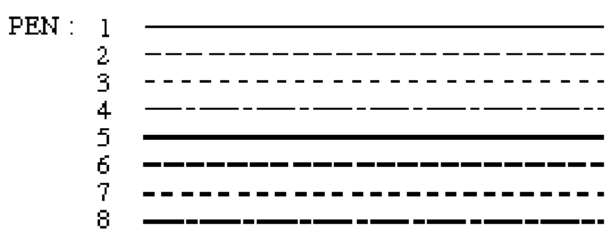
Plot commands are implemented so that you can build from Gifa any kind of plot by adding each plot element to a plot file. So each plot command requires a parameter which is the filename in which the plot is stored. There are also context commands, which do not realize any plot actions, but rather describe how the next plot will be done (for instance `CX`)

CX, CY, ROTATE, PLOTTER, CONFIG

The 3 first commands determines the kind of plots that will be performed by the plotting commands. The size of the plot will depend on the contexts `CX` and `CY` (in centimetres). `ROTATE` exchange X and Y axes on the plotter such that the drawings are rotated on the sheet. Two kinds of plotter can be connected to Gifa : a HP-GL plotter (usual for pen plotter) or a Postscript (usual for laser printers). The plotter is chosen with the `PLOTTER` command, you can tell for which plotter the program is currently connected to with the `CONFIG` command.

PLOT, PEN, PLOT, PAGE, PLOTOFFSET, title, PLOT?, FORGET

The `PLOT` command will plot whatever is currently on the screen. In 2D, the plot will be strictly equivalent to what is displayed by the `CDISP2D` mode; in 1D, the plot will be equivalent to what is displayed, but in a `CX` x `CY` format; in 3D the last extracted plane, as seen on the 2D display will be plotted.
`PEN` permits to change the active pen. In HP-GL, this is the number of the pen; in Postscript, 8 kind of lines are available :



`PCOLOR` permits to choose a colour when plotting on a colour Postscript printer. Only the 8 basic Gifa colours are thus available. If you wish to use more exotic colours, you should edit the plot file itself (look at the macro `setfont` for instance).
`PAGE` will send the page to the plotter, and eject the page on a plotter.
`PLOTOFFSET` is the constant offset on x and y axes which is applied for each plots. Each plotting command will see the point at coordinates 0;0 as actually being offsetted from the true 0;0 of the paper with the `PLOTOFFSET` values. `PLOTOFFSET` permits to stack different plots on a single sheet.
`title` will plot the text following the command at coordinates x=0, y=CY+1.
`PLOT?` will prompt you for all the parameters currently used for plotting.
All these commands will prompt you for an output parameter, entering `*PL` (or `*PLOTTER`) will output the plot to the plotter. Entering a file-name will create a file containing the graphic commands for the plotter. If you send several plot

commands to the same file, the following commands will be appended to the first one in the plot file, thus permitting to make composite plots on a single sheet. The `PAGE` command appends the order for page change, send the file to the plotter port, and makes Gifa « forget » about the plot file, thus plotting again on that file will erase the file and start a new plot. `FORGET` will only makes Gifa forget the file, without sending it to the plotter.
The plot file can also be sent to the plotter by typing at the operating system level :
$gifaplot plot_file plotter_type
with plotter_type being either postscript or HP-GL, depending on the type of plot file you have created.
When working in postscript, it is very convenient to use a Display Postscript program to monitor the state of the current plot file.

PLOTAXIS, PLOTAXIS?, plot_damp

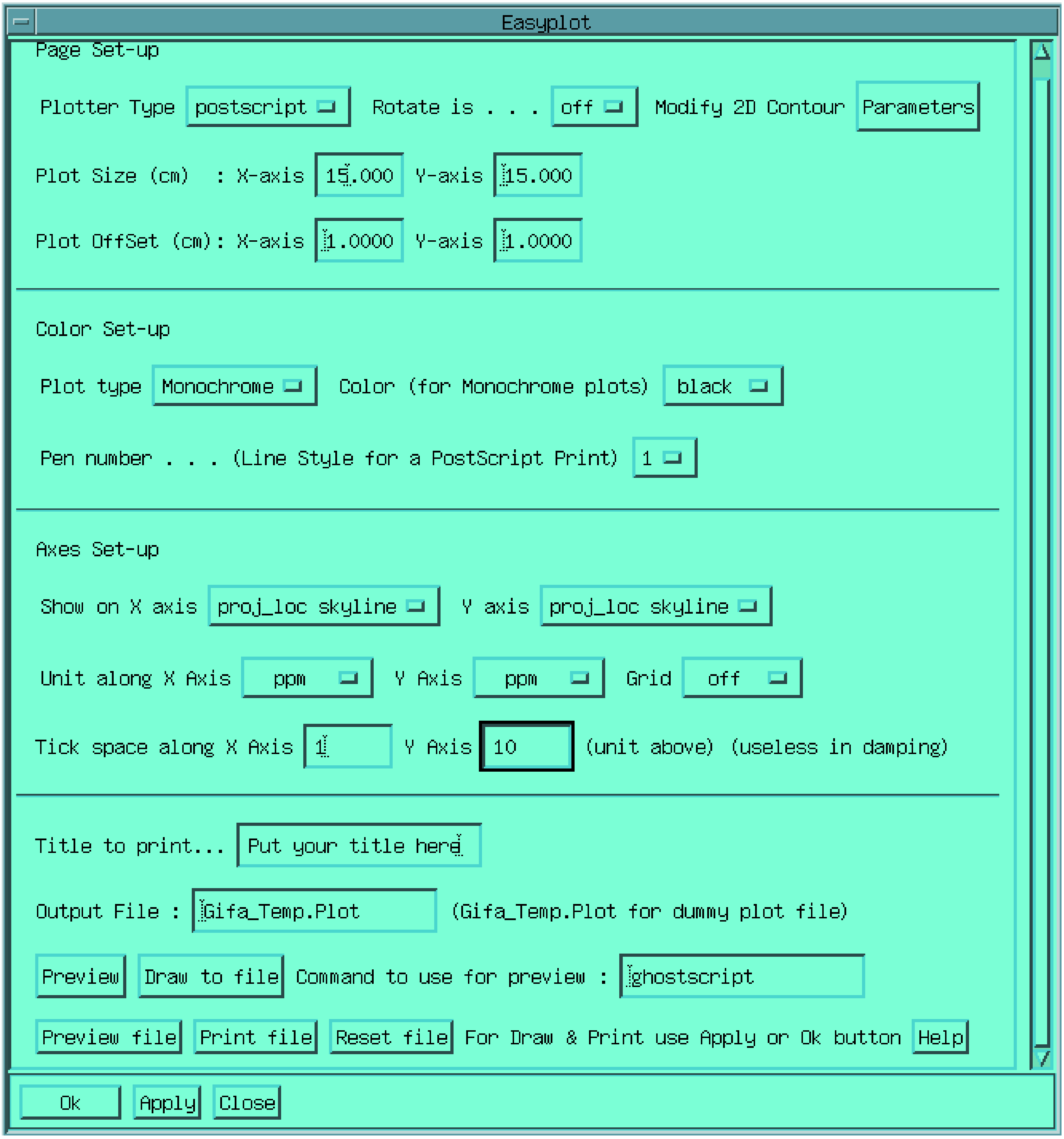
The first command permits to draw an horizontal and/or vertical axis on the current plot. The graduation is done according to the current values of `SPECW` and `OFFSET`. `PLOTAXIS?` permits to configure the axes drawn by `PLOTAXIS`. `GRID` permits to draw a grid of CX by CY on the current plot, it will use the axes determined by `PLOTAXIS?.` Check the macros plotn and nice_plot for examples of these functions.
The macro plot_damp draws on the plotting file a logarithmic scale, to be used only for damping (DOSY or Relaxation) processings.

STPL, STPL?

`STPL` will generate a stack plot either on the screen (`*S`), on the plotter (`*PL`) or in a file. The stack-plot depends on the value of the following contexts :
`CX` : length in centimetres of a line.
`CY` : maximum height of a peak in centimetres.
`SCALE` : scaling applied to the data before plotting, if scale=1 then the larger peak on the surface will be CY high, if scale>1 then clipping will occur.
`STDY` : each new line is offsetted by `STDY` centimetres in the Y axis.
`STSKIP` : every `STSKIP` line of the data-set will be drawn.
`STSHIFT` : each new line will be shifted right by `STSHIFT` points, if negative then the shift is done on the left. (May be fractional).
`STSKEW` : determines how the horizontal lines are skewed during plot, (if negative skewed to the left and to the right if positive.
`STPL?` permits to check all the parameters in one command.
On screen stack plots are currently limited to 256x128 points (larger plots generally crashes the graphic).

easyplot

This macro has been written in order to help the user in realising rapidly simple plots. A FORM shows up which permits to determine most of the plot parameters for a 1D or 2 2D plot.



Easyplot

Page Set-up

Plotter Type: postscript — Rotate is . . . off — Modify 2D Contour [Parameters]

Plot Size (cm) : X-axis 15.000 Y-axis 15.000

Plot OffSet (cm): X-axis 1.0000 Y-axis 1.0000

Color Set-up

Plot type: Monochrome — Color (for Monochrome plots): black

Pen number . . . (Line Style for a PostScript Print): 1

Axes Set-up

Show on X axis: proj_loc skyline — Y axis: proj_loc skyline

Unit along X Axis: ppm — Y Axis: ppm — Grid: off

Tick space along X Axis: 1 — Y Axis: 10 (unit above) (useless in damping)

Title to print...: Put your title here

Output File : Gifa_Temp.Plot (Gifa_Temp.Plot for dummy plot file)

[Preview] [Draw to file] Command to use for preview : ghostscript

[Preview file] [Print file] [Reset file] For Draw & Print use Apply or Ok button [Help]

[Ok] [Apply] [Close]

Most controls are natural, and refers to to parameters which have been presented above. However, some controls may have to be explained:

- Only the currently zoomed region will be plotted.
- If you switch from postscript to HP-GL and define large CX and CY, it is better to close and reopen the easyplot form.
- Axes set-up uses the the PLOTAXIS set of commands to draw the axes on the spectrum
- Output file: can be anything, if GifaTemp.Plot is chosen (it is the default) the file will be removed after plotting

- preview commands :
  The form makes use of a preview program to display the resulting plots before actually doing the plot. The name of the command to use can be changed, by default the ghostscript display postscript program is used. The associated controls are :
  - writes to a temporary file and starts a preview for that file.
  - **to file** sen the drawing to the defined file. You can add several drawing to the same file.
  - **file** starts a preview on the current drawing file.
  - **File** send the file (created with the Draw to file) to the plotter, and start a new plot.
  - **File** undo every thing and start a new file.

SEVERAL BUFFERS AVAILABLE

Several buffers are available in Gifa. The three main buffers (for 1D, 2D and 3D) are chosen with the DIM command. Those 3 are the only one on which generic processing is available.
Other buffers are available :

DATA, EXCHDATA, ADDDATA, MULTDATA, MINDATA MAXDATA

DATA Is a generic buffer designed to be a « second hand ». It can hold 1D, 2D or 3D data-sets, accessed with `GET` and `PUT`. You can also exchange the content of the working buffer with the content of DATA, sizes should match in this case.
The current buffer can also be modified according to the content of the `DATA` buffer with the `ADDDATA`, `MULTDATA`, `MINDATA` and `MAXDATA` commands. `ADDDATA` and MULTDATA respectively add/mult the content of the `DATA` buffer to/with the current data-set. `MINDATA` and `MAXDATA` leaves in the current data-set, at each data point, the smallest (respectively largest) of the `DATA` buffer and the current data-set; they can be used to create home-made, fast symmetrisation macros. All these commands modify only the content of the current data-set, and leave the `DATA` buffer untouched.

TAB, FILTER, WINDOW

are special purpose 1D buffers. They are designed for specific actions :

- TAB contains the series of X values, when the current 1D buffer is considered to hold scattered Y values. This permits to do scatter plot (SHOWLINEAB command) and is used by several other modules (such as `FITGENE` or INVTLAP).

- `FILTER` holds an apodisation function, used with the `APPLY FILTER` command (only if the `FILTER` context is set to 2). In 2D or 3D, F1, F2 and F3 domains will be sequential in the buffer. You can design an exotic apodisation function, put it in the `FILTER` buffer, and use it.

- `WINDOW` is the description of valid points within the data-set (more precisely of $\frac{1}{\langle\sigma\rangle}$). Thus a null value in `WINDOW` indicate a point with total uncertainty. `WINDOW` usually holds 0.0 or 1.0 entries, but any real values are valid though negative values have little meaning. The command `WINDOW` permits to design the `WINDOW` function; by resting it to 1.0, or by « digging » holes in it. `WINDOW` is used by `BCORR 3`, `MAXENT`, `FITGENE` etcÉ It is useful also to put to zero a certain region in a data set (for instance to remove the water curtain in 3D).

However, you might use them to simply GET and PUT, if you are searching for additionnal hands. Be carefull though not to erase important information which was already held in there.
Other buffers are available, used by the MaxEnt or the line-fitting package, see the specific documentation.

PUT, GET, SHOW, APPLY

are used to manipulate the different buffers.
`PUT` (P) loads the given buffer with the current data-set
`GET` (G) brings back the given buffer as the current data-set
`SHOW` (S) displays the given information in the 1D window or in the 2D window
`APPLY` (A) computes the result of the mathematical operation.

The buffer :	**can be** :	**S**	**G**	**P**	**A**
WINDOW	window used to compute the chisquare in MaxEnt processing, also used by the polynomial mode of BCORR	*	*	*	*
TAB	small buffer used to hold tabulated value, used by the general fitter, and the MaxEnt inverse Laplace transform.	*	*	*	
FILTER {n }	Generic filter function, also used for MaxEnt Deconvolution	*	*	*	*
DATA	data used as a second hand by MaxEnt and Linear Prediction, also used as a general purpose buffer.	*	*	*	
LAMB	the evolution of Lambda during MaxEnt iteration	*	*		
ENT	the evolution of Entropy during MaxEnt iteration	*	*		

CHI	the evolution of ChiSquare during MaxEnt iteration	*	*		
STEP	the evolution of Step during MaxEnt iteration	*	*		
SUM	the evolution of Sum of point of Image during MaxEnt iteration	*	*		
CONV	the evolution of Convergence during MaxEnt iteration	*	*		
RESIDUE	The residue after a MaxEnt run	*	*		
LINEFIT	The result of the last line fitting	*	*		
AMOEBA	the contours used for integration during the last 2D Paris integration	*	*	*	
FT	The causal Fourier transform (FTBIS) of the current data-set	*			
CURRENT	the current data-set (useful for comparing with SHOW)	*			
PLANE Fi n	the nth plane of the 3D data-set, along axis Fi (F1, F2 or F3)			*	
ROW n	the nth row of the 2D data-set			*	
COL n	the nth col of the 2D data-set			*	

The command `SHOW` uses, for some option, the value of the context `SCOLOR` to determine the colour to be used by the display.
The two commands `GET DATA` and `PUT DATA` permit to put aside a data set for a while and getting back to it very quickly. Note however that the size of the larger data-set that can be put aside this way is only a fourth of the larger Gifa data-set.
The `PUT FILTER` command (to be issued in 1D mode) has a syntax which depends on the setting of the `NCHANNEL` context. `NCHANNEL` describe how many independent channels will be considered in the filter window. If `NCHANNEL` is 1, then the current data-set will become the filter function. If

`NCHANNEL` is greater than 1, then the command will prompt you for which channel to load the filter function in. This permits to build a 2D or 3D filter function (in which case, the i channel corresponds to the i dimension); or to build multichannel deconvolution functions for MaxEnt. If the channel index 0 is given, then the action is as in 1D.
The command `PUT` permits to put the content of one lower dimension buffer into a higher data-set. You can thus `PUT ROW` index or `PUT COL` index in 2D or `PUT PLANE` index in 3D :

```
Gifa> ROW 1 DIM 1 MULT 0.5 DIM 2 PUT ROW 1
```

will divide by 2 the first row of the data-set.

DISPLAYING AND PLOTTING 3D DATA-SETS

Plane by Plane

It is possible with Gifa to display different planes extracted from the 3D data-set, but also to display the 3D data-set as a volume in a 3D manner.
Plotting planes extracted from a 3D consists simply in selecting planes with the `PLANE` command, and plotting them as 2D with PLOT. For instance the simple macro :

```
for i = 1 to $si1_3d
plane F1 $i plot *pl title ("plane #"; $i) *pl page *pl
endfor
```

would do the job.

Displaying and Plotting 3D Volumes

It is possible to display 3D pictures of 3D data set. The principle is to draw a series of contour plots for each axes in a 3D space. This kind of display is useful for checking the quality of a 3D data-set, and also for making nice pictures.

DISP3D, REF3D

`DISP3D` will open a window devoted to 3D display. No picture is displayed when opening because of the time a 3D display usually takes to compute. Unlike the 1D and 2D display, the 3D display must be forced with the `REF3D` command, and will remain unchanged even if the data or the parameters are changed. As usual ^C permits to stop the 3D display being computed.

CX, CY, CZ, ALPHA, BETA, GAMA, AXIS3D, ZNOT, OFFSET3D, SCALE3D

This commands determine the aspect of the 3D display. The volume size is described by the `CX, CY, CZ` contexts. When opening the 3D window the size is taken to be equal to the largest of the 3 contexts. `ALPHA, BETA` and `GAMA` are the angles which describe the view point. `AXIS3D` determines which planes will be contoured. A value of F123 describes a complete contour, but simpler display (and faster) may be chosen. Usually a F1 value is the fastest choice. `ZNOT` is the focal with which the volume is displayed. A large value corresponds to a « tele » position, a small value to a « wide ». `OFFSET3D` determines the position of the 0 point, values range from 0 to 1. `SCALE3D` is a scaling factor applied to the final image.

DISP3D?, CHECK3D

All these parameters can be easily entered and checked with the `DISP3D?` macro. An interactive, graphical mode is provided with the command `CHECK3D`, which display interactively an empty cube, thus permitting to modify the main ones.
Buttons are available with the `CHECK3D` command, which permits to directly choose some typical points of view (along each axis, along the main 3D diagonal of the cube). See above the definition of the box in the Graphic User Interface manual part.

PLOT3D

This command generate on a plot file a plot equivalent to the display obtained with the `REF3D` command. The plot file must then be closed with the PAGE command, see the chapter on plotting.

Strip files and Strip plots

A set of macros have been designed to handle strip files. This can be performed for all kind of 3D, even if examples will be given here for double resonance experiments.
The principle is to extract strips from the 3D where you know (from a previous 2D, or from the projection) there is signal, and to construct from these strips a pseudo 2D data-set. This is done here by using a 2D peak picking for locating strips to be extracted.
Imagine you have a 3D ^{1}H-^{15}N NOESY-HSQC experiment from which you want to create the strip file, (say your ^{1}H dimension are F1 and F3, and the ^{15}N dimension is F2), here how you could do.

- Get a nice HSQC plane, by using the adequate projection from the 3D (F1 projection)
- go in 2D mode and make a peak-picking of this plane, check with SHOWPEAKS that all your peaks are there.
- if it's not done join your 3D (yes strips work only on JOINed 3D, no big deal, simply write your memory-located 3D and JOIN it !) and start the strip_file macro, it prompts you for the axis to strip down (here F1, and the starting and ending index of the peak in the table to use.
- you get a 2D where each entry in the 2D peak table has been projected as a F1 strip. The spectral width and frequency of the fake F2 dimension have been adapted so that in ppm unit, you will have the peak index in the 2D peack table as a ppm coordinate.

You may prefer to use a real 2D HSQC to make the peak picking, (with, say, more resolution) the processing is the same, but simply start with the 2D, and make our peaking. Just be VERY carefull that the ppm calibration is EXACTLY the same than the 3D, since every thing will be computed in ppm.

With the same technique, you can create strip plots with the strip_plot macro, an additional information to be given is simply the number of strips per page.

WORKING ON FILE RATHER THAN IN MEMORY

Introduction to the cache system

Up to now we have only seen how the processing was performed on the data-set currently held into the main memory. This way of working is fast and efficient for small data-sets, but inefficient for large data-sets. So a capability has been put into the Gifa program to work on file rather than on memory. It is thus possible to process much larger data-set, that would not fit into the main memory. This is performed through a cache-memory system that is implemented into the Gifa program. This features has the double advantage of permitting the processing of very large data-set (no limitation in size, as far as the software is concerned), and to speed-up the processing of the processing of large data-sets that can be done otherwise in-memory.
With Gifa V4.0 the cache system has been fully rewritten, in order to extend its capabilities, and reliability. Most of the limitations that were in the previous version of the cache have been removed. You should also notice a large speed increase when working on large files. However, the user interface has been kept as much as possible unchanged, except for the `GETC` and `PUTC` commands which have now a syntax more similar to other Gifa syntax.

Detailed Principle of Operation

The cache memory works on the standard file format (accessed also through the `READ` / `WRITE` commands). It is based on two principles :

- A block structure of 2D and 3D data set files, that permits random access of data in any direction,

- A memory area that is devoted to minimising the number of disk accesses (the cache-memory system).

In the previous version of the cache (Cache version 1.0, in Gifa 3.x and in pre-release of Gifa 4.0), the blocks were of a fixed size of 4096 words (16 kbytes) corresponding to 16x16x16 in 3D, to 64x64 in 2D and to 4k in 1D. This is no longer true, in the present version (Cache version 2.0, since Gifa 4.0), the blocks are adapted to the experiment and to the computer. This means that the block may take any value, optimised for the current hard-ware (typically 4kbytes and 16 kbytes), and that the division of the blocks will depend on the sizes of the experiment, in order to optimise access speed in all the spectroscopic dimensions.

The standard format features also a header which holds all the parameters of the data (such as dimensionality, sizes, spectral widths, etc...). This header is in text format, and can easily be displayed with a more command. The user can easily add his own information in the header with the `GETHEADER` `PUTHEADER` commands. The header is of a fixed size equal to the size of a data block. The cache system can be used with several files in the same time.

Cache memory access is much faster than a disk access. The block structure of the file speeds up the processing of large data sets. For instance to access 2 successive planes of a 3D, the first plane will be loaded from the disk, and then the second will be subsequently held into the cache memory. There is no real limitation of the size that the cache system may handle, however each file opened with the cache system will use room in the computer memory allowing to fit several line (plane) of the 2D (3D) experiment.
It is important to note that writing onto the cache is not equivalent to writing onto disk. There is some mechanism, that will store on disk the content of modified block when needed; but the content of the file is not warranted when working through the cache system (this is very different from the WRITE command). This has no effect when working from within Gifa itself, since all file access will go through the cache system that will insure the coherence of the data. However it may have effect in certain cases such as :

- the file from another program (may be another Gifa);

- failure of the computer;
- bug in Gifa (?).

When needed, it is possible to « flush » the cache and to copy to disk all the modified blocks with the commands `FLUSH` and `FLUSHCACHE`.
Processing data-sets with the cache memory system usually requires using some macro for scanning through the complete data-set for the operation to be completed. A set of macros is provided which will permit an efficient and easy processing (see below).

Commands for using the Cache

Working with the cache system consists in creating a file in standard format (with `WRITE` or with `NEWFILEC`), connecting to the file without actually reading the file (with `JOIN`), and applying the processing either row by row (1D and 2D) or plane by plane (3D).

JOIN, DISJOIN, LISTFILEC

The command `JOIN` permits to connect the program to a standard file format, without actually loading any data into memory. The effect is to load the contexts that describe the connected file (such as size, dimensionality, itype, etc... see below the variable paragraph). Several files can be `JOINed` independently, the contexts will always hold the parameters of the last `JOINed` file. `DISJOIN` will disconnect the program from the currently connected file, any modified data on the data-set will be saved onto the file. `LISTFILEC` output the list of the currently `JOINed` file.

dataset, GETHEADER, PUTHEADER

`dataset` lists the value of the contexts describing the last `JOINed` data-set. `PUTHEADER` permits to specifically modify a parameter of the currently connected data-set, the modification is directly stored to the file(after a `FLUSH` or a `DISJOIN`). The parameters handled by Gifa (as returned by dataset) can be modified, but any parameter can be put into the header with this command. `GETHEADER` permits to read the value of parameter in the file header. The read value is available in the `$c_header` variable.

GETC, PUTC

This two commands permits to move data back and forth between the file and the main working memory.
`GETC` loads data from the file to the memory; `PUTC` copies the content of the memory to the file. Both commands have a similar syntax. They permit to handle data areas as well as complete lines, planes and cubes. The action taken depends on the dimensionality of the `JOINed` file as well as the value of `DIM` in the Gifa working context.

```
dimensionality of the JOINed file :
```

value of dim :	1D	2D	3D
1D	1D area	1D area	1D area
2D	not applicable	2D area	2D area
3D	not applicable	not applicable	3D area

general syntax is :
```
GETC / PUTC low up
```
in 1D, where low and up determines the area to load, or
```
GETC / PUTC axis ... index ... low up ...
```
in 2D and 3D where the number of axes, indexes and coordinates depends on the kind of transfer. See per command manual for the detailed syntax.

SHOWC

This command permits to display a currently `JOINed` data-set, without actually loading it into the main memory. All the current display parameters are used for the display, but the scale which has to be defined to the command. The coordinates of the current zoom window used for the display is converted to ppm, and used for the display of the `JOINed` data-set. This permits to display spectra acquired in very different conditions.

The `SHOWC` command does not actually load the whole data-set in memory for displaying, plays game with the cache memory. This is why it is slower than the regular display.
This command is used in the `super1d` and `super2d` macros which permit to overlay several display on screen.

FLUSH, FLUSHCACHE

The `GETC, PUTC` commands do not read and write data directly from the disk, but from the cache memory. If some data are modified, the cache system takes the burden of updating the file when needed. However, in certain cases, it might be needed to have an updated file.
`FLUSH` flushes onto disk the modified data corresponding the currently `JOINed` file. `FLUSHCACHE` will flush all the file currently `JOINed`.

NEWFILEC

This command creates a template for a standard file format, and reserve the room for the data. The command prompts the user for all the parameters that will be needed to create that file. It will be then possible to fill that file with the `PUTC` command. Note that the file created with the `NEWFILEC` command are in 'write only' mode. This strange mode consist to a file on which only `PUTC` is available, and in writing blocks on the file without checking if data were already present. This is fine as long as you scan regularly the output file with a `for i =1 to $c_size..` loop. Thus random writing on such files, even though not forbidden, produces wrong results.

READC, WRITEC

This two commands have been already seen in a previous paragraph. They are strictly equivalent to the `READ WRITE` command. They could have been developed as macros, using the `JOIN` and `GETC` commands for `READC`; and `NEWFILEC` and `PUTC` for `WRITEC`.

Using macro : proc2d proc3d proj3d easy2d

A set of macro is provided to process on file data : `proc2d` and `proc3d` in `/usr/local/gifa/macro`.
Each command requires the name of the input file, the name of the output file, the axis to process and the commands to apply.

- proc2d :

```
proc2d in_file out_file axis 'list of commands'
```
process the data row by row or column by column depending on axis (either F1 or F2). You can also use proc2d in interactive manner, being prompted for each value. In this latter case, when entering the list of commands, you can use several lines, finishing the last empty line with a ^D. The commands are regular Gifa commands, in 1D mode. Macro are valid.

- proc3d :

```
proc3d in_file out_file axis 'list of commands'
```

is equivalent to `proc2d`, but processes the 3D in a plane wise manner. Be careful that the command you enter will be in 2D mode, and that whatever plane you choose for the processing of the 3D, the commands will refer to the plane as F1, F2.

- proj3d :

Computes the projection of the JOINed 3D data-set. One of the 3 axes F1, F2 or F3 should be chosen, as well as the projection algorithm.

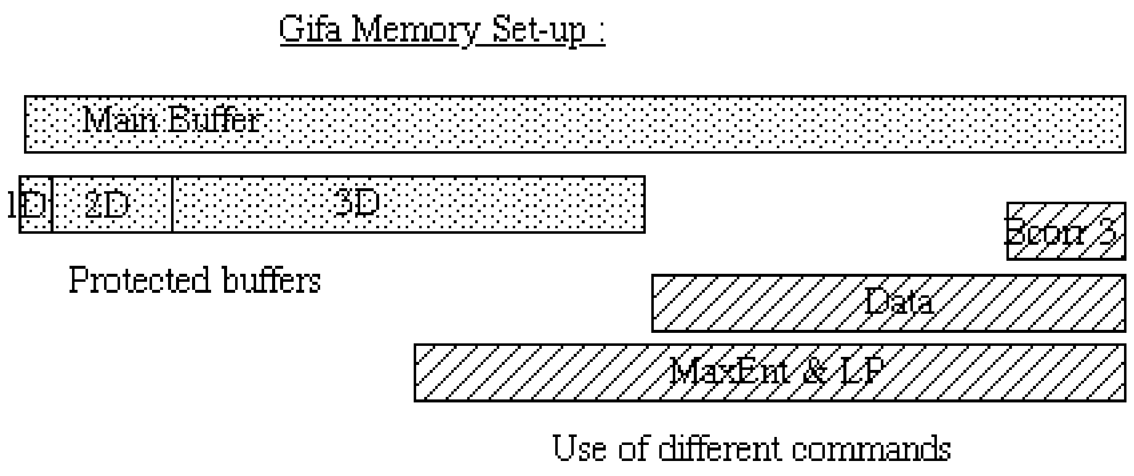
Note that the macro `easy2d` will switch by itself to on-file processing if the file is too large to be processed in memory.

UNDERSTANDING THE MEMORY SET-UP

The Gifa program holds all the data in one single large memory buffer. This buffer is used for several purposes, and may be divided into smaller pieces. The size of this buffer is displayed when entering the program, or with the `CONFIG` command. There is no way to use a larger data-set than this memory size but recompiling. This buffer is used for 1D as well as 2D and 3D operations. In all cases the whole buffer is available. However, when moving back and forth between 1D, 2D or 3D mode, or when using memory intensive commands, only partial regions of the buffers are protected. The size of these protected regions are given with `CONFIG` command. The idea is that you can eat-up all the available memory for a single data-set if you wish, but that certain operations will be forbidden on it.

For instance, you can handle a full memory 2D data-set if you do not wish to do 3D. However, when working in 3D, if you zero-fill a 2D plane extracted from the 3D, over the protected area size for 2D, you will destroy a part of the 3D buffer. You will sometime get the question : 'This will overflow the xx buffer, Ok?' when there is any risk of destroying one of the buffer. This question is not asked during macro execution, where you are supposed to know what you are doing.
With the current set-up, the size of the protected 3D area is typically 1/2 of the size of the main buffer, the larger protected 2D is 1/4 of the larger 3D, and the protected 1D is 1/4 of the larger 2D.

On another hand, certain operations in Gifa need large work storage, and will use the top of the main buffer for this; thus being incompatible with a large data-set. These commands are : Maximum Entropy, the linear prediction package, the automatic baseline correction `BCORR 3` and the `PUT DATA` and `GET DATA` operations. However the amount of memory used depends on the command. The Maximum Entropy and Linear Prediction (but not the `BURG, READC` and `WRITEC` commands which are in-place) will use the 3/4 of the main buffer so only 1/4 will be left for regular processing; this limitation is independent from the size of the larger data-set to be processed by MaxEnt which is 1/8 of the main buffer. The `PUT DATA` and `GET DATA` command will use 1/2 of the main buffer. The `BCOR 3` command will need only 1/8 on the top of the main buffer. With all these commands the remaining of the main buffer can be safely used. If you try one of these command with a too large data-set in the buffer, the data-set will be corrupted on the overlapping region.



If you feel that the program is too small for your needs, contact the person who installed the program on your machine, and ask him to install a larger definition of the program . Definitions for 1 Mega, 4 Mega and 16 Mega are in the distribution.

SIMULATION OF NOESY SPECTRA

The two commands SIMUNOE and CHEMS permit to generate simulated NOESY spectrum from intensity computed from the 3D structure of the molecule. First a list of chemical shifts should be constructed, either directly or with the help of the CHEMS command. The chemical shift list is a file with one entry per line, each line holding the name of the atom (in PDB-like format), the chemical shift in ppm, and the line-width. Then the command SIMUNOE will use this file and a intensity file constructed with the help of the CORMA program (Keepers & James J.Magn.Reson.
The command generates an output file containing information on all the peaks in the spectral window. This file is very useful when searching for the origin of peak seen in the simulated spectrum. For this purpose, if you specify a null size for the simulation, then no data will be generated, and the data-set currently held in the memory will not be over-written, but the output file will be created, thus permitting to generate peak files for small spectral region.
The commands `SIMUNOE` and `CHEMS` used to be needed for the simulation of NOESY data-sets, however these commands were quite buggy, and have been superseded by a simple set of macros which realizes the same thing.
`SimSpect2D` is the basic command, it takes as parameters : first a data-base of all the spins along with their chemical shift and line width; then a list of intensities in a simple free format, finally a set of controls, determining the 2D modulation and whether the data-set is symmetrical or not. This macro will generate a 2D FID, that can be then processed as a regular data-set. Be careful however, that the process can be quite lengthy, if you compute a large region, with a lot a peaks and a lot of points.
The chemical shift data-base is in dbm format, and can easily be built from an ascii file with the `mkdbppm` macro. The intensity file is in ascii, and can have been generated by any program. For instance, the *CROWD* program developed in our laboratory can create NOESY and ROESY simulation from 3D structures and dynamic information. However the SimSpect2D macro can be used to simulate any kind of 2D data-sets.
There is an additional macro available : `SimSpect2D_form` which creates a form permitting to very simply enter parameters for the `SimSpect2D` macro.

PEAK-TABLES, PEAK-PICKING LINE-FITTING AND INTEGRATION, THE PARIS MODULE

The Gifa program has a complete capability to detect, integrate, line fit and manipulate peaks.
This facility is based on an internal structure holding information on the last peaks detected. This internal structure is called the peak-table. 3 such peak tables are simultaneously held in the program, respectively for the 1D, 2D and 3D data sets. Peak tables can be loaded, listed, read and written onto disk, and peaks can be selectively removed form the table. The commands relative to the peak table always refer to the current peak table, as defined with the `DIM` context.
The peak table is used by the peak-picker module, integrator module, the line fitting module and the linear prediction module.

MAX, MINIMAX, PEAK

These commands permit to perform an automatic peak picking of the peak in the current data set (1D, 2D or 3D).You have first to choose a "value-window" which will be used by the peak-picker to select

peaks in the data-set, the `MINIMAX` command permits to select the upper and lower bound for this window.
One way of doing is by searching for the largest and smallest points in the data-set with the MAX command, which set the default values for `MINIMAX`. However, the smallest value has usually to be reset by the user to a more realistic value. For instance you can compute the mean level of noise with the `EVALN` command, and enter the noise level time a given scalar as the minimum intensity for a peak :

```
point ;select an empty area
max evaln %% minimax (4*$noise) % ; loads the value
```

The command `PEAK` will then find all the local maxima which lies within the upper and lower bounds in the data-set, and load the peak table. It will search for peaks only in the currently defined ZOOM window. The peak table will restrict its search to the currently displayed spectrum, thus permitting to perform a peak-picking on a restraint area of the spectrum by zooming at it. When using `PEAK` in 2D and 3D, you will be prompted for a packing radius. Giving a non-zero value has the effect of "packing" or "linking" all the peaks which are less than n points apart from each other into the larger one, thus removing the entries of the smaller ones from the peak output.
The macro `peak_pick` has been designed to help in this process, and is called from the GUI.

Viewing : REFPEAKS, pklist, SHOWPEAK, SHOWPEAKS, PLOTPEAKS,

These commands are the basic commands for displaying the peak table.
`pklist i` *`j`* will list the contents of the current peak table to the screen from peak *i* to peak *j*.
`pklist %%` will list the complete peak table. The origin of the peak table (picker, integrator, LP, etc...) is given, and all the descriptors of each peak. The unit used for the coordinates of the peaks depends on the context `UNIT`. This command can be successfully used with the `CONNECT` - `DISCONNECT` commands to generate listings. It is a macro, so can modify it to fit you specific needs.
In the Peak menu, `REFPEAKS` is used instead of `SHOWPEAKS`, in order to display, at each time the screen is refresh, the peak table. The commands `SHOWPEAKS` and `PLOTPEAKS` display respectively on the screen or on the current plot, the content of the peak table. `SHOWPEAK` permits to highlight a specific peak in the peak table, by drawing a cross. `SHOWPEAKS` and `SHOWPEAK` uses the current definition of `SCOLOR`.

Modifying : PKSELECT, PKRM, pkrmi, pkrmz, PKCLEAR, PKCLEAN, PKRESET, POINT->PK, SETPEAK, SETPEAK2

These commands are the basic commands for the modifying the content of the peak table.
`PKSELECT` permits to select specific entry into the peak table. Non selected entry will be lost.
`PKCLEAR` removes all entries from the peak table. It is thus equivalent to `PKSELECT 0`. On the other hand `PKRM` permits to remove a single entry in the current peak table.
The two macros : `pkrmi` and `pkrmz` have been designed to graphically help the user in removing peaks. `pkrmi` remove one peak, clicked by the user; `pkrmz` removes all the peaks located within one

region.
`PKCLEAN` permits to remove entries in the peak table with intensities smaller than a given value.
`PKRESET` reload the intensities in the peak-table, as found on the data-set.
`POINT->PK` adds the content of the point stack (see above) to the current peak table. This permits to interactively add missing peaks in the peak table.
`SETPEAK` and `SETPEAK2` are other commands for modifying the content of the peak table : the parameter of the peaks can be manually entered with these commands. `SETPEAK` permits the user to enter all the parameters of the peak, while `SETPEAK2` requires only the coordinates.

Storing : PKREAD, PKWRITE, PKRESET

These two commands permits to read and write peak tables on the disk. The files created are in text format one peak per line in free format. When reading with `PKREAD`, the values read can either be added to the current peak table, or used as a new peak table. `PKREAD` loads all the values as stored in the file, thus the intensities are also reloaded, the command `PKRESET` permits to compute again the intensities from the peak position. `PKRESET` is also useful when the data set has changed.

PKPROJ, PKSYM

These commands permit to perform mathematics on the 2D peak table. `PKPROJ` will load the 1D peak table with content of the 2D peak table projected along one dimension. `PKSYM` will symetrise the 2D peak table either removing or adding non symmetrical values.

Integrating : INTEG, MSKINTEG, mskread, mskwrite, MSKMODIF, MSKCONC

`INTEG` integrates all the peak found in the peak-table. This is an implementation of the PARIS algorithm (V.Stoven et al. J.Magn.Reson. 82-1). The integration of a peak is performed by finding a contour spanning the largest extension of the peak (the amoeba); the sum of the points under this amoeba is then computed. The defined amoebae are stored as a matrix within the program.
The amoeba is determined by four criteria, with four parameters associated : RATIO, SLOPE, THRESHOLD, and RADIUS. The first criterion that will trigger will determine where the extension of the amoeba should stop.
RATIO triggers when the ratio between the largest point in the peak and the current evaluated point gets below RATIO.
SLOPE triggers when the slope changes. A value of 0 will be triggered anytime the slope changes from negative to positive (thus starting to climb on another peak); a larger value will permit more freedom on the slope.
THRESHOLD will trigger whenever the evaluated point is below the (absolute) value of THRESHOLD.
RADIUS determines the maximum extent of the amoeba from the central peak.
When using the integrator, the noise level and the systematic offset of the surface should have been evaluated with the `EVALN` commands
There are two additional contexts that determine fully the PARIS module : `SIGN_PEAK` tells the peak-

picker if the peaks are to be found either as positive peaks or as negatives peaks. `ZERO_QU` tells the integrator that the amoebae should be computed on the absolute value of the surface, (but the integrator will still work on the normal surface). This is very useful when working on NOESY spectra where there is zero-quantum coherences signals (the integration of which is zero).
The `SHOW AMOEBA` command shows the amoebae that have been found at the last integration step.
The `MSKINTEG` will integrate the peaks as defined by the current peak table and mask (amoeba) matrix. This command permits to integrate several experiments using the same amoeba definition. The amoeba matrix can moved around with the `PUT` and `GET` commands. The 2 macro `mskread` and `mskwrite` permit to read and write directly amoeba matrices along with peak tables.
`mskread` and `mskwrite` are 2 macros meant for storing on file and retrieving the current peak and amoeba definitions.
The amoeba can also be modified with the `MSKMODIF` and `MSKCONC` commands which permit respectively to set a given pixel to a given peak (or to remove it from the amoeba definition), and to concatenate two amoebae.

Line fitting : LINEFIT LINEFITD

These commands start a line fitter, based on a Levenberg-Marquardt minimiser, convergence is determine either by the number of iteration (context `ITER`) or by the size of the step (context TOLERANCE). Fitted line can be either Lorentzian or Gaussian, as chosen by the parameter of the command LINEFIT. The content of the peak table is used as starting values, and the result of the fit is stored back in the peak table. The quality of the fit is estimated with a χ^2 value, which is computed as the sum of the residues : $\chi^2 = \frac{1}{n}\sum_i \sqrt{\frac{(y_i - Y_i)^2}{\sigma_i^2}}$

Where Y is the recomputed spectrum, y is the current spectrum and σ_i^2 is the variance of the noise, estimated from the NOISE command. Thus a correct fit corresponds to a final χ^2 equal to 1.
Optimized parameters are returned as updated values in the peak table. Error bars are computed from the covariance matrix computed during the fit. Values and error bars are available as contexts for further processing. Note that error bars are equal to two times the standard deviation estimated from the covariance matrix, thus corresponding to 95% confidence limit. If you prefer the 68.3% confidence limit, divide all error bars by 2.
Results can be examine with the standard commands `SHOW LINEFIT` or `SHOWPEAKS`. As an addition, macros called `show_fit` and `plot_fit` are provided, which permit to display/plot a composite display of the current data set with the fitted lines superimposed on the spectrum.
All the values extracted during the fit are actually stored into the peak table. All the fitted parameters are stored back as the peak parameters, as welll as the error bars on the fitted values. The peaks (or quantities) which are not fitted stay unmodified.
The command :

```
put data get linefit mult -1 adddata
```

Permits to obtain the residue (that part of the data which is not fitted), the command

```
get data
```

returning to the current data-set.

The `LINEFITD` (linefit detailed) command permits to finely select which peak and which parameters will be fitted, and which will not, for instance fitting only the amplitude in a series of relaxation measurements, or fitting only the frequencies in a titration.

SUMREC

is a simpler integrator that will integrate on a rectangular area determined by the user. You can use point to select the integration area.

INT1D

Is a simple graphical integrator for 1D data-sets, similar to the old CW mode. Its actually replaces the contents of the 1D buffer with the running integration of it.

THE GENERAL FITTER

In addition to the line-fitting module presented in the previous chapter, Gifa contains a generic, multipurpose, general minimiser. This module is able to minimise any function on a set of parameters. The minimiser works with the Powell method, which does not require derivative expression. It relies on a two steps minimisation which are controlled with ITER (Number of iteration in the outer loop) and MINITER (Number of iteration in the inner loop, execute for each axis, and for each outer iteration). Values of 10 for both control seems to be Ok. note that if only 1 parameter is to be optimised, only one outer loop is needed, then ITER is not used, MINITER is then the only relevant control. This explains also why the minimisation is much faster when only one parameter is to be minimised.
Functions to be minimised are written in the Gifa language and should simply be a regular Gifa expression.
The general minimiser comes in two flavours: MINIMIZE and FITGENE. MINIMIZE is a general minimiser, FITGENE is a general Fitter,.

MINIMIZE

This command takes a given expression and try to minimise it's value by varying some free parameters in it. The expression is given in Gifa syntax, and the free parameters are the global user variables $P1, $P2, etc...
You give to the command i) the expression to be minimised (as a string) ii) the number of free parameters to be adapted (called $P1, $P2, ...)
The command returns the minimum found (also available in $chi2)
e.g.

```
MINIMIZE 'abs(sin($p1)/$p1 - 0.5)' 1
```

returns

```
MINIMIZE Final Value : .27782464E-04
```

and p1 is set equal to 1.89543
This tells you that the function sin(x)/x is equal to 0.5 when x = 1.89543
Note that $P1, $P2,.. are global user variables. If they exist when the command is called, their values will be used as initial trials, if they does not exist, they are created and set to 1.0

FITGENE, showexp

This command permits to fit a given function to a set of experimental points Xi, Yi. Yi is taken to be the regular 1D buffer, Xi is obtained from the TAB buffer (see Buffers). This permits to fit an arbitrary function through any set of X,Y points.
You give to the command i) the expression of the function to be fitted (as a string) the running parameter is called $X ii) the number of free parameters to be adapted (called $P1, $P2, ...)
FITGENE then minimises a chi2 and returns its value after fitting (also available in $chi2)
e.g.

```
FITGENE '$p1 + $p2 * $x' 2
```

realises a linear fit of the data points.
The standard macro showexp permits to draw the given expression to check the quality of the fit :

```
showexp '$p1 + $p2 * $x'
```

will actually draw the fitted line.
Again, the $P1, $P2.. $Pi are global user variables that can be freely used after the fit. FITGENE will also set the variables $DP1, $DP2..$DPi which contains the size of the error bar for each fitted parameter. Note that error bars are equal to two times the standard deviation estimated from the covariance matrix, thus corresponding to 95% confidence limit. If you prefer the 68.3% confidence limit, divide all error bars by 2.

Note also that the expression to be fitted is a generic string, and can for instance, very well be held in a (global) variable :

```
set exp := '$p1*exp(-$p2*$x)'
fitgene $exp 2
showexp $exp
```

will fit T2-like data-sets

SPECIAL AND GENERAL PURPOSE COMMANDS

help apropos

`help` is a macro, it permits to general info on a specific item. `help` with no arguments gives you the list of the commands available.
`apropos <word>` is a very convenient macro that scan all the helps files searching for a given word. It permits to search for some information without knowing where to start from.

LOG_FILE CONNECT DISCONNECT

In permanence, all the input generated by the user, and the output generated by the program are journaled in a file called gifa.log. This file can be either kept or removed when exiting the program. At any time the user may redirect the journaling to another file with the command : `CONNECT` file_name. The program will then create a file called file_name where all the journaling will go. The command `DISCONNECT` will resume the journaling to the gifa.log default file, and close the previously `CONNECTed` file. If the command `CONNECT` is issued while a file is already `CONNECTed`, the former file will closed, and the new file will be opened.

EXIT, QUIT, or BYE

are the normal exit of the program. These commands ask you whether you want or not to keep the log file which as been built during the processing and which contains a copy of all the interactive during the session. This file is called gifa.log. On UNIX system, be careful to rename it (mv command) before rerunning Gifa otherwise the saved log file will be erased by the new log file.

SIMU, SIMUN, ONE, ZERO

SIMU simulates a complete experiment as a set of exponentially decaying sines plus noise in 1, 2 or 3D. Noise can also be added to the simulation
SIMUN is different, it permits to simulate only one line, but this line is added to the current data-set, with all the current parameters (spectral width, sizes, etc...). The command ADDNOISE permits to add a Gaussian noise to the current data-set.
The commands ONE and ZERO put respectively the value 1.0 and 0.0 in the current buffer. Very useful for initialising a data-set before SIMUN, or for visualising an apodisation function.

SHOWLINE, SHOWTEXT, PLOTLINES, PLOTTEXTS, PLOTLINE, PLOTTEXT,

are commands that permit to draw a line (xxxLINE) or to write a string (xxxTEXT) on the screen (SHOWxxx) or on the plotter (PLOTxxx). The first 4 commands take coordinates in index on the current data-set. They will both draw according to the zoom state. SHOWxxx commands will use the value of the context SCOLOR as the colour. PLOTxxx command will also depend on CX and CY. The 2 last commands take coordinates in cm.

SHOWPATTERN, plotpattern

permits to draw a given pattern on the srceen. Crosses, squares and circle are available. Coordinates (position and size) are given in index on the current data-set. SHOWPATTERN is a hard-wired command for speed optimisation, when working in the assignment package. on the other hand, plotting is done with a macro, and tend to be rather slow.

SHOWLINETAB

Is different from the precedent command as it uses the content of the TAB[] and working 1D buffers for rapidely drawing a set of vectors. TAB[] is used as the X coordinates (interpreted in various unit) and the working 1D buffer is used for Y coordinates. The number of point to draw, and the precise location on the drawing on screen have to be precised.

^C

The control C key will abort the process in progress and bring you back to the prompt level (on VMS machine and most UNIX machines). This may sometime take a few seconds before executing the abort.

TIMER

is a context that when set to one will activate the display of elapsed and cpu time taken by every command. Useful for benchmarking.

VERBOSE and DEBUG

These 2 contexts will generate verbose output from some module in Gifa. For instance `VERBOSE` will detail the processing of Maximum Entropy run, of macro files, of baseline correction, of fitter evaluations etc...

SH, Unix commands

The SH command will send its parameter to the operating system. For instance you can type :

```
" ; on VMS machine

; on VMS machine

Gifa> sh "ls -l /usr/data"
```

You can also type SH alone, this has the effect of creating a sub process at the operating system level (csh is used), you then get back to Gifa by loging out (^D on UNIX).
Using SH, several macros have been created that mimic UNIX : more, rm, ls, vi, pwd, etc... There are also two special editing command : `vip` will edit in your $HOME/macro directory, and `vim` in /usr/local/gifa/macro

Note that the sh() function is also available, it returns the first line of the output of the command.

CD

`CD` *`dir`* permits to change the current working directory to *`dir`* . Equivalent to UNIX. Note that this is very different from :

```
sh 'cd dir'
```

which actually creates a sub-process which executes cd, thus having no effect on the current job.

FREQUENTLY ASKED QUESTIONS

Q : How do I refer to Gifa in my publication ?

The main paper presenting the current version of the Gifa program has recently been published, the reference is :

- Pons, J.L., Malliavin, T.E. and Delsuc, M.A., 1996. Gifa V4 : a complete package for NMR data-set processing. *J. Biomol. NMR*, 8, 445-452.

Before this recent reference, the first reference of a paper completely devoted to Gifa was :

- Delsuc, M.A., 1989. A New Maximum Entropy Processing Algorithm, with Applications to Nuclear Magnetic Resonance Experiments. In: J.Skilling (Ed.), Maximum Entropy and Bayesian Methods, Cambridge 1988, pp. 285-290, Kluwer Academic, Dordrecht.
  which describes the GIFA MaxEnt algorithm/implementation

You may also use the following references :

- For DOSY processing:
  M.A.Delsuc et T.E.Malliavin (1998) Maximum Entropy Processing of DOSY NMR Spectra - *Anal Chem* **70**-10 p2146-2148

- for the assignment module :
  T.E.Malliavin, J.L.Pons & M.A.Delsuc An NMR assignment module implemented in the Gifa NMR processing software. (1998), *Bioinformatics* **14-7** p624-631

- for the J-Deconvolution method7
  Marc A.Delsuc and George C.Levy.(1988) J-Deconvolution: the Application of the Maximum Entropy Processing to the Deconvolution of Coupling Patterns in NMR. *J.Magn.Reson.* **76** p306-315

- generic texts on use of MaxEnt
  M.A.Delsuc, M.Robin, C.Van Heijenoort, C.B.Reisdorf, E.Guittet and J.Y.Lallemand.(1990) Application of Maximum Entropy Methods to NMR Spectra of Proteins. NATO Workshop Il Ciocco.
  M.A.Delsuc, P.L.Fortier, C. van Heijenoort, T.E.Malliavin, M.Robin, A.Rouh (1992) Le traitement des donn}es en RMN , *les Cahiers IMABIO* **3** p49-61

- MaxEnt in 3D
  M.Robin, M.A.Delsuc, E.Guittet and J.Y.Lallemand (1991) Optimized Acquisition and Processing Scheme in 3D NMR Spectroscopy *J.Magn.Reson.* **92** 645-650

- for the Hyper Complex Fourier transform
  Marc A.Delsuc (1988) A New Spectral Representation for 2D NMR Spectra: The Hypercomplex Numbers. . *J.Magn.Reson.* **77**, p119-124

- Data compression, the READZ WRITEZ commands
  Th}r•se E.Malliavin, Marc A.Delsuc, Jean-Y.Lallemand (1991) Compression of Multi-dimensional NMR Data-sets , *J.Magn.Reson.* **94** p 630-634

- the SMOOTH command
  P.L.Fortier, M.A.Delsuc, E.Guittet, P.Kahn and J.Y.Lallemand (1991) Convolution Difference in the Time Domain, and its Application to 2D NMR *J.Magn.Reson.* **95** p166-169

- the Build-up curve processing part
  Th}r•se E.Malliavin, Marc A. Delsuc and Jean Y.Lallemand. (1992) Computation of Redfield Matrix Element from Incomplete NOESY data-sets *J.Bio.NMR.* **2** p 349-360
  Christine Reisdorf, Th}r•se .Malliavin et Marc A.Delsuc (1992) Accurate estimation of inter-atomic distances in large proteins by NMR ; *Biochimie* **74** p809-813

- Baseline correction, The BCORR 3 command
  Alain Rouh, Marc-Andr} Delsuc, Gilles Bertrand, and Jean-Yves Lallemand (1993) Baseline correction of FT NMR Spectra : An Approach in terms of classification , *J.Magn.Reson.* **A-102** p357-359

Q : I get the message - Licence is NON-VALID - ?

Guess what, your licence is not valid! If you already registered, then check again the installation procedure. If you are not registered, just contact me (Marc-Andre.Delsuc@cbs.univ-montp1.fr) I will ask you to sign a licence agreement, and you will get a licence key.

Q : I get the message - No graphic possible - ?

You did not connect correctly to an X-server display. Gifa is perfectly able to run without X-window, but obviously, all the graphic commands won't work. In the case described here, the standard startup.g macro stops when trying to set-up the graphic environment. To set-up the X-window environment, do (in csh) :
setenv DISPLAY the_name_of_your_X-terminal:0.0
if you use a remote work-station for displaying, check that you enabled the remote display by doing : xhost +.
To work in graphic-less mode, create your own startup.g (in HOME/macro or in local directory (.)) which will take precedence over the general startup.g.

Q : Gifa starts correctly but menu nor graphic window show up ?

If it does not complains about no graphic available, but that actually no spectral window nor menu show up, it is most probably that the standard environment is not available. Gifa is such that it relies a full set of files to perform correctly. These files should be located in the standard place: /usr/local/gifa. If there are absent, check your installation, it could be due to the fact that your forgot to download the gifa_basic.tar.Z archive.

Q : I get the message - Killed - and Gifa does not start ?

This is a typical message when the available memory on the machine is not sufficient to handle a big program. Try -to use a smaller version of Gifa (There should be 3 sizes on the distribution kit), -to extend the swap area of your machine.

Q : I get the message - Cannot open the gifa.log file - ?

This message means that Gifa could not create the gifa.log journaling file in your $HOME directory.

When running, Gifa copy all the commands to this file. This file permits to redo a processing, or to find the result of a previous one. When exiting, you are asked for keeping or removing that file.
Gifa cannot create the journaling file in several cases :

- a gifa.log file is already present in your HOME. This happens when you choose to keep the file when exiting, if a gifa is already running for the same account, or if a previous run of gifa exited with a crash.
- the disk is full, or your quota is exhausted
- the environment variable $HOME is not defined, or miss assigned, (happens when using su).

Q : How do I compare spectra in absolute display scales

Each spectrum in Gifa is displayed relative to its larger point, the parameter SCALE describes how this larger point will appear on screen, SCALE = 1 means that the larger point will be full screen. To make absolute display (and plots) you need to force the program to scale to the same larger point for display. The value of the larger point is called ABSMAX. when the data are changed, or when set to 0, it is recomputed as the largest point in the data-set. But you can change it by setting its value to any non-null positive value. Thus using the same ABSMAX for 2 different data-sets will result in absolute display.

Q : How do I set a plot level relative to the noise level?

Often one wishes in 2D, to have the lower plot level set relative to the noise level (the 3 sigma case). The noise level can be computed with the EVALN command. Then the simpler is to put ABSMAX to the value of the noise (thus telling Gifa that the larger point is at the noise level (a bit strange I agree)), then to set SCALE reminding that the lowest level is 32 times lower that the higher level.
Thus, if you want a 3 sigma plot :

```
EVALN x y z t ; evaluate the noise
absmax $noise ; set absmax to the noise
scale (1/(3*32)) ; set scale
```

Q : Why are spectra completely shifted in super1d/super2d

Those 2 macros are based on the SHOWC command which works in ppm coordinates. Thus to be able to superpose spectra, you should have correctly calibrated all your spectra. Note also that an earlier bug in ux2cach was making Gifa files with all spectral parameters wrong (before version 4.05b).

Q : How do I transfer data from my spectrometer to Gifa ?

There are several answers to this question, which depend on the kind of spectrometer you use and the nature of the link.

- Varian

No problem there, there is a READV command in Gifa to access directly the Varian files, there is even a set of macros to extract spectral parameters from the `procpar` file : `varian_param`; and to give a graphic user interface to it : `varian_read.` You can switch to Varian mode to have these as ypour standard GUI.

- Bruker DMX - AMX

Use the ux2cach utility (in gifa/util/ux2cache) which convert UXNMR data files (not the pdata) into native Gifa files.

- Bruker AM/WM

This is always a problem, because of the difficulty to get out of the Aspect computer. An additional problem is that the Aspect computer stores data on 24bits, instead of the 32 bits modern computers use. Some utilities are given here, but expect to have some tuning to do because of the numerous options available.

using NMRLink

Try to use the nmrlink program, the source is in util/moul4

using Bruknet

Try to use the program in util/bruknet

using Lightnet transfer

Try to use the transdata; program, the source is in util/moul3

- Other cases

There are several possibilities :
¥ The simplest way is to write Ascii files, and load them with the READT or READM command. Use the WRITET / WRITEM command to get an example of the correct format (most parameters are optional).
¥ If you use MATLAB, there is a READM command for you.
¥ You can look into the gifa/util/ux2cache where you will find the library for accessing the native Gifa file format, and the source of the utility which converts UXNMR files into native files (Again, most parameters are optional). There is also the older gifa/util/ux2gifa utility which converts into the

FTNMR compatible format (the READH command) which is somewhat simpler to implement, but much less powerful.

Q : I am a Varian user, but the FT seems to be tuned to Bruker - ?

You are actually right, the program is currently developed in a group equipped exclusively with Bruker machines so far. But, bear with me, you are not out of luck. You have noticed that the possibility to read Varian files is implemented in the menu interface, what about the processing ?
A complete set of macros are available in /usr/local/gifa/macro/varian which realizes the equivalent of the standard processing, but for Varian data-sets.
Simply choose the Varian mode in the mode menu, better yet, put the following line into your startup.g file, And you start directly in Varian mode..

```
SETPATH ('/usr/local/gifa/macro/varian' ; $GIFAPATH)
```

Q : I get the message - Size too big for operation - ?

with the bcorr 3 commands for instance.
These command use alternate buffers which are not available because of the size of the current data-set. You can : i) choose a bigger version of the program (there should be three in the distribution) memory allocation is static in Gifa. ii) choose another algorithm. For instance remember that

```
chsize (%*2) ft phase x y real
```

and

```
ft phase x y ift ftbis
```

give the same data, however the second method requires twice as small buffers.

Q : What is the - Overflow xxx buffer - message ?

Gifa handles the data in several buffers that overlap (see "UNDERSTANDING MEMORY SET-UP"). when the data gets too big some of the less needed buffers are used for handling the data. Thus certain operations becomes not available. See precedent Question.

Q : Why am I sometimes prompted for the overflow and sometimes not ?

When a buffer is going to be overflowed by the current command, and when the command is issued from the main level (from the prompt or from a menu/form) then you (the user) are asked if it is OK to overflow. The command is aborted if you answer no. This question is not asked when the command which creates this overflow is issued from within a macro. This permits to write macro that will always work. If you want to protect from within a macro, you should make the test in the macro.

Q : My spectra show up completely scrambled after FT ?

There several data format possible for NMR : in 1D, data can be real, complex, or acquired in the sequential "Redfield trick" mode. in 2D and 3D, data can be in tppi, in States-Haberkorn, in gradient N+P interleaved, in phase-modulation modes, or even in a mixture of these. Complex parts can be interleaved or separated, there are different conventions on the sign of the imaginary parts; etc... etc... There is a set of macro which has been designed to deal with this problem : ft_sim and ft_seq (for 1D or acquisition dim processing) ft_tppi ft_sim and ft_sh_tppi for nD. These macros work without problems for Bruker/UXNMR spectra, however they might need some tuning for another set-up. These macros are built from simple commands, there are many possibilities in Gifa, try to play with FT RFT FTBIS; REVF INVF REVERSE; SWA USWA. Once you have found a set-up, you might want to propagate it in the macros ft_* found in the distribution.

Q : What is the analytical counter part of the SIN command ?

the exact definition of the SIN command is :
with the parameter X [0.0 0.5] and N points to process
s = 2*(1-x)
w = PI/((N-1)*s)
phi = PI*(s-1)/s
after the **SIN x** command, the ith point of the current buffer is multiplied by :
SIN(i) = sin((i-1)*w + phi) with i : 1..N

Q : What is the analytical counter part of the GM command ?

the exact definition of the GM command is :
with the parameter GB, N points to process, a spectral width of SW
Z = ((GB*PI) / (4*SW*SQRT(LOG(2))))^2
after the **GM GB** command, the ith point of the current buffer is multiplied by :
GM(i) = exp(-Z*(i-1)^2) with i : 1..N

Q : How does SIN or GM relate to Bruker equivalent ?

Or actually the opposite, how can I keep SIN or GM equivalent to the Bruker manner?
Indeed the definition of the parameters are VERY different.
Well, first you should forget Bruker, but then, if you are really addicted, you may try the `sin_bruker` macro which implements the Bruker SIN/SSB command; and the `gm_bruker` macro which does the Bruker GM command. You may also look into the macro code to see what are the analytical to transform from Bruker to Gifa.

Q : How can I start Gifa in background job ?

Check on the writtin macro documentation.

Q : Plot does not work

Gifa builds plots by adding to a file the different graphics to be plotted. The command PAGE has the effect of closing the plot_file (equivalent to FORGET) and to send the plot_file to the plotter with the shell script 'gifaplot'. This shell script is copied into /usr/local/bin at installation (check that it is in your PATH), and should be adapted to your particular set-up. A very common reason why plots do not work is either that the shell script has not been adapted. This shell script is called with 2 parameters : the name of the plot_file; the type of plotter (HPGL or postscript). As sent, it is configured to use lpr, and to remove the file if it is called Gifa_Temp.Plot. Another reason is when for some reason the internal memory of plot-files, and the state on disk are different (for instance if a write fails, or if CD is used), in this case, remove the corrupted file, and use FORGET to clear the internal counter part.

Q : set si1_2d = 2048 does not work

Gifa internal variables are sometimes a bit confusing. They look like user variables when you fetch them, however you cannot write into them. In the case of the question above, $si1_2d has to be changed with CHSIZE. Actually, the command :

```
set si1_2d = 2048
```

creates a user variable, with the (unfortunate) name si1_2d, which will 'hide' the internal variable. Next time, when you will evaluate $si1_2d, you will get the value of your user variable (in this case 2048), not the size of the current 2D, which is no more available.

Q : SH just returns, and do nothing

This happens when the memory is very loaded on the machine, and that the fork() call fails. Try to : remove useless processes; use a smaller version of Gifa; expand the swap area (or the physical memory) of your machine.

Q : my log file does not go away when I exit with : exit n

Same as above (the exit n command internally uses the SH mechanism)

Q : What is the Gifa data format

The fundamental file format (READ command) is a bit complicated to describe, but the library for accessing it is fully available in util/ux2cache/cache_mad.c in the distribution. This is a library, which permit all accesses (1D, 2D, 3D), the format is also described. This code has been made public domain.
There are also data format which are easier to handle for a small program :
ft-nmr kind or format (READH); ascii format (READT); matlab format (READM).

Q : How can I read Data set as text?

There are several ASCII format input available in Gifa, they correspond to several READx commands

(you have the full list if you do help write)
READM is a matlab compatible format (-ascii format). It consists in raw data (without any parameters); numbers are formatless; 1D is one single line; n (F1) p (F2) 2D is n lines of p entries.
READT is a generic ascii format; header entries are available so you can put parameters; numbers are formatless, one per line, after the (required) keyword **data:**
n (F1) p (F2) 2D is nxp lines of 1 entry
load is even more generic, (it is a macro)
no parameters, one entry (formatless) per line, only for 1D (slow !)

In any case you never need two columns, entries are assumed to be sampled regularly, and the SPECW parameter give the sampling frequency. You can also use the respective WRITEx commands to see what the input files should look like.

Q : Planes displayed from 3D require very unrealistic scale

3D processing is usually handled by on-file processing. There is a bug in the set of command permitting to realize this (probably in NEWFILEC) which can perturbate the value of the Absmax parameter of the file (which hold the value of the largest point, and is used for display). The macro `reset_absmax` permits to restore the correct Absmax value.

ACKNOWLEDGEMENT

The Gifa program is the result of a constant effort going in several NMR labs in France : It started about 10 years ago in I.C.S.N. (Gif-sur-Yvette), in Ecole Polytechnique (Palaiseau) and is now developped in C.B.S. (Montpellier). I want to thank here Pf. J.Y.Lallemand, Pf.P.Potier, Pf J.M.Lhoste and M. Kochoyan for their help in the direction of these laboratories. This program has been made available because of the help of a lot of people, either in development or in using and debugging the program, and this, either in my lab or in other laboratories.
In first place I want to thank T.E.Malliavin, J.L.Pons, who have developed large parts of Gifa, as well as M.Robin, A.Rouh and V.Stoven who were involved in the earlier development of this program.
I also want to thank all those who helped me in this project (either contributing small parts of it, helping the port to new architecture, or giving access to their machine for the development and port to new platforms : S.Auge, J.Basque, Y.Bernier, F.Billois, F.Bontemps, L.Caussade, F.Capozzi, G.Deleage, C.van Heijenoort, C.Labadie, F.Lacourt, L.Ladaviere, S.Lavaite, R.Legoas, C.Pruvost, G.Salnikov, G.Zhu (and all the ones I forget !).
And all the people which helped me by enjoying, using and debugging it.

I hope that you will have fun, and enjoy working with the Gifa program. In any case don't hesitate to contact me (bug reports and propositions are specially welcomed).

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