THE Gifa PROGRAM.Version 4.0

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A complete Package for NMR Processing

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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-André Delsuc. Please contact :

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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 such as Maximum Entropy processing or Linear prediction. 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.

This version V4.0 is now in final version, however it is evoluating all the time, check your ftp server ! This version is distributed under a licence. There is no fees for academic laboratories, however 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 the following address : ftp://tome.cbs.univ-montp1.fr/pub/gifa_v4 .

Previous released versions have been : 1.0 (Initial VMS Version), 1.1 (revised version), 2.0 (first port to UNIX), 2.1 (first stabilised version), 2.5 (introduction of linear prediction, polynomial baseline correction), 3.0 (introduction of macro-language, on-file processing, etc...), 3.1 (new peak-picker and line-fitter), 4.0 (Motif version, new user interface, new language capabilities, new cache, extended line fitter). Several versions have been used internally in our lab, and may have been released by mistake.

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).

•Fast Fourier transform (direct and inverse; real, complex, and hypercomplex). Hilbert transforms.

•Zero-filling and truncation.

•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 :

* 2'30" on Macintosh Centris 650 - running MachTen
* 37" on SUN SparcStation 2
* 31" on IBM Risc 6000-320
* 17" on HP 725/50
* 15.5" on SGI-INDY PC

* 12.6" on IBM Risc 6000-560
* 12.3" on SUN Sparc 20
* 10.4" on SGI-INDY R4400
* 7.5" on HP 735/99
for the complete processing of a 512x2048 data points data-set, including :
-exponential windowing in F2, shifted sine bell in F1.
-hypercomplex FT with zero-filling in F1 and phasing in both axes.
-cubic 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)

•Addition, multiplication of data-sets.

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.

•Multi-windowing facilities : up to 4 active windows in the same time, many passive windows.

•Fast zoom mode - Fast interactive phasing mode.

•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 :

•Maximum Entropy processing of 1D as well as 2D data-sets. A generalised 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…

•Integrated processing of NOESY build-up curves, permitting to accurately evaluate distances.

•Automatic peak-picker in 1D 2D and 3D; Automatic peak integrator in 1D and 2D.

•Line fitting of mixed Lorentzian and Gaussian Line Shapes

•Several file formats are available, notably a FT-NMR® compatible format, a MATLAB® compatible format, a compressed format, a generic file format, permitting direct random access, and several others.

A Complete set of Macro :

•A complete graphic user interface written in the macro language

•Calibration, integration, peak-picking, etc..

•Fast interaction with the mouse on 2D and 3D

•Help for attribution, on screen and on plotter

•Easily extensible with the control language

The User Interface is characterised 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 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).

•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 (don't panic, just type EXIT to get out of it!) . 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 and a horizontal menu bar 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.

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 consists in sets of related commands, arranged in vertical button boxes, each such boxes being called by clicking the associated button in the menu bar. Each button box can be opened and closed at will.

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` button box (the box will show off if you hit the `File` button in the menu bar), you will get a short introduction.

Entering

```
Gifa> HELP
```

at the prompt level will give you the same message. The command HELP is here in uppercase, it can actually be entered also in lowercase, or even in a mixture of upper and lower case letters. 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)!

The HELP command 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 command which permits to determine the current unit used on the data-set : PPM, Hertz (as determined form internal parameters) or Index (ranging from 1 to n in the case of a data-set of length n), or seconds (for time domain data-sets).

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.

You are now ready to process your first data set.

BASIC GRAPHIC USER INTERFACE

The standard graphic interface is characterised 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 and Zooming

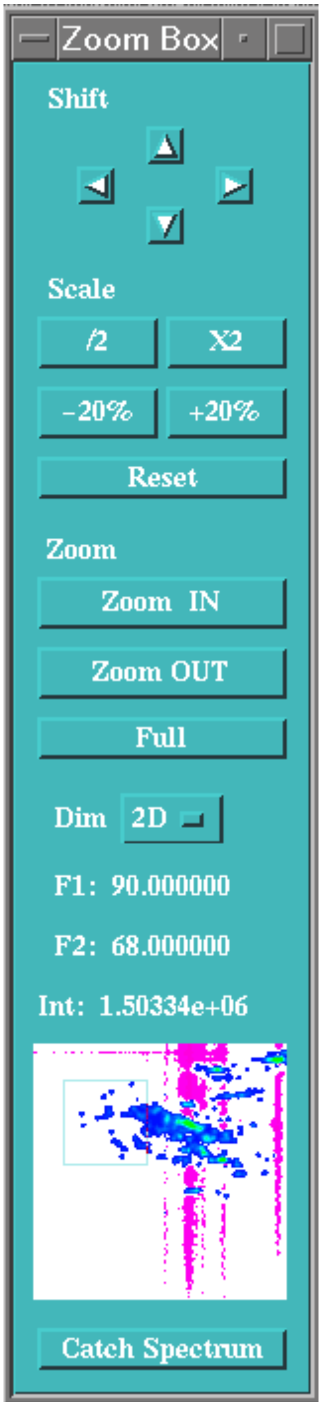
Several graphic windows can be opened at the same time within Gifa. By default, when entering the program, a 1D display and a 2D density display window are opened. Several other graphic windows can also be opened (see CDISP2D, DISP3D, FREEZE). The data held in the working buffers are shown in these windows.

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 colours in these windows can also be modified with a set of colour commands.

All the spectral windows can be FREEZEd, 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 any-more.

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.

A control box 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)).



To zoom the display, simply click on the graphic window with the left and middle buttons pressed, and draw a rectangle on the display. You can redraw as many time as wished this rectangle. To zoom into the selected region, simply click in this rectangle with the left and right button of the mouse. You can also use the Zoom in and Zoom out buttons in the control box. The spectrum showed in this box, is the complete spectral region, as was dispayed when you clicked on the Catch Spectrum button. The white rectangle in it, shows the current zoom region.

The four little arrows 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 pop-up menu Dim, can be used to rapidely switch between the 3 working buffers : 1D, 2D and 3D. Finally, the text above the small spectrum is the current coordinates of the mouse, that you get whenever you click in the display.

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.

However it 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 necessitate additional files for interactive processing or for texts, these files are held into the /usr/local/gifa/macro/gm directory.

If a menu is buried below other windows, clicking on the menu name will pop the menu again.

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.

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 ressemble 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.

File menu

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

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.

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 command 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.

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

Convert from UXNMR

This button calls the shell script ux2cach.sh which permits to convert from a Bruker/UXNMR file format (acquisition data, not the processed data) to the standard Gifa file format. The command first prompt for the directory in which the data resides (for instance /u/data/guest/nmr/your_exp/1) and then to the Gifa file format. It will then ask for information which cannot be found in the Bruker files.

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 command.

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 command.

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 (mad@cbs.univ-montp1.fr) a short bug report.

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.

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

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.

... 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.

...Linear Prediction

Will add a menu permitting Linear Prediction processing.

... 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.

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 is 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.

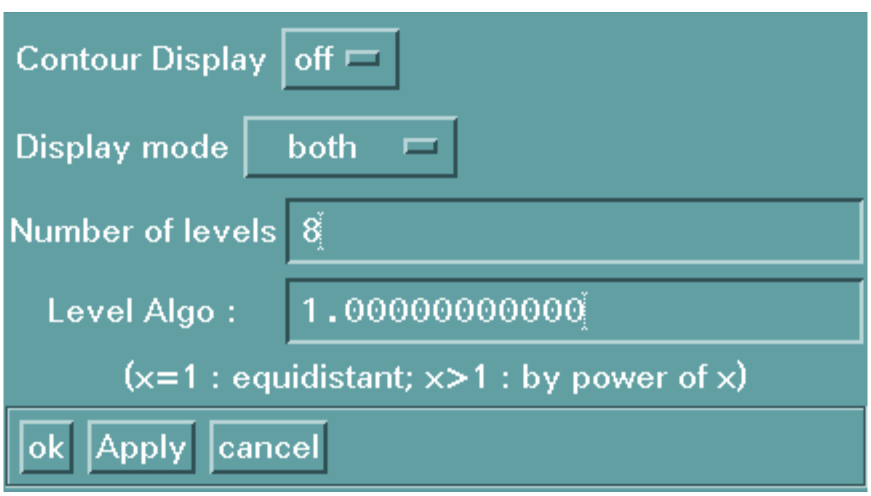
Zm (Zoom Control)

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

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.

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.

store zoom

Clicking this will memorize 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

Rzoom

When in zoom mode, this button will jump to symmetrical zoom region, relative to the diagonal.
This button is equivalent to the RZOOM command.

super1D

Creates a form box which permits to display up to 2 additional 1D spectra on the top of the current 1D sprectum held in memory
Equivalent to the super1d macro

super2D

Creates a form box which permits to display up to 2 additional 2D spectra on the top of the current 2D sprectum 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 (SCLAE, 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

A independent buffer is available, which can hold indifferently a 1D, 2D or 3D data-set. This buffer cannot be 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 or ppm. Equivalent to the `UNIT` command.

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.

<u>Processing</u>

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 <u>Proc 1D</u> menu.

<u>Em...</u>

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.

<u>Gm...</u>

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.

<u>Sin...</u>

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.

<u>SqSin...</u>

As the <u>Sin</u> button but applies a squared sine-bell. Equivalent to the SQ`SIN` command.

<u>Tm...</u>

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.

<u>Correct 1st point</u>

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.

<u>ChSize...</u>

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.

ZeroFill

Extend the size of the current data-set to a size equal to the next power of two.

ft_Seq

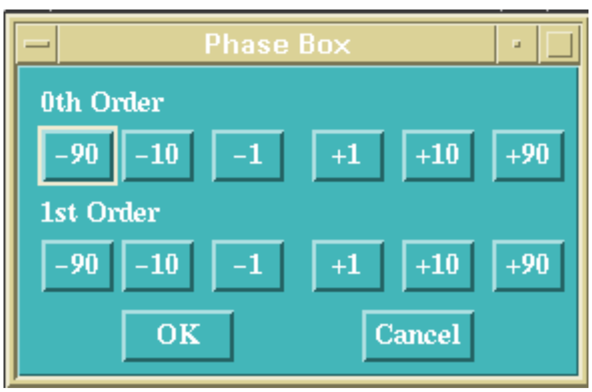
Realises the Fourier transform suitable for a data set acquired in *sequential* mode : real and imaginary part alternatively sampled. Equivalent to the `ft_seq` macro or to the `REVF RFT` command.

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.

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 commandsprompt 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.

ZeroFill F1 - ZeroFill F2

Increases the size of the dataset in the F1 or F2 domain up to the next power of 2.

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.

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.

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 promt you wether 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 promt you wether you want a "Skyline" (keep the highest points) or a "Mean" (sum all points) projection. Equivalent to the PROJ F2 command.

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 additionnal 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 differesnt 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.

<u>Largest Set</u>

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

<u>ZeroFill F1</u>

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

<u>ZeroFill F2</u>

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

<u>ZeroFill F3</u>

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

<u>Burg3d</u>

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

<u>ft_Seq (F3)</u>

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

<u>ft_Sim (F3)</u>

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

<u>ft_tppi (F2)</u>

<u>ft_sh (F2)</u>

<u>ft_sh_tppi (F2)</u>

<u>ft_tppi (F1)</u>

<u>ft_sh (F1)</u>

<u>ft_sh_tppi (F1)</u>

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.

<u>Phase</u>

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

<u>Real...</u>

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

<u>Real F123</u>

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

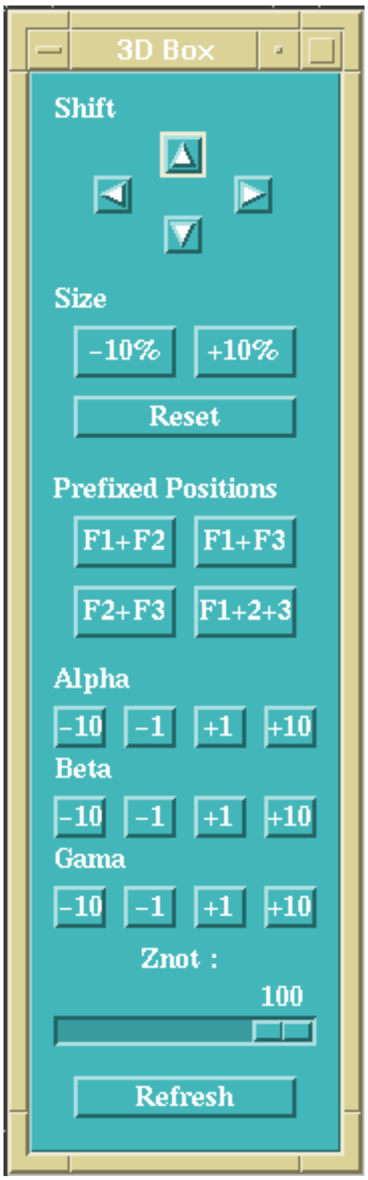
Opens the 3D display window, equivalent to the `DISP3D 1` command.

parameters...

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

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* buttom 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 examinate 1D spectra by clicking on a orthogonal 2D plane.

planeint

Starts the `planeint` macro which permits to interactively examinate 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 the **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 ile, processed in memory as regular 2D 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 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 intance it can usefull 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.

get region

This ones permits to load in the central memory a portion of the currently JOINed data-set. You will be prmpted 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.

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 finaly 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. 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

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.

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. (stil experimental - the menu I mean, the commands are fully operationnal)

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 promt 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 "urg 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 spectm.

Cadzow proc.

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

PKlist

Actually prints the content of the peak table. Equivalent to the PKLIST %% command.

Plot menu

This menu holds all the entries for realising simple plots.

Easy plot

This button launches a from which permits to determine all the parameters for a standard plot, with axes, grid, choice of colours, etc...

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 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://tome.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 pick (pp)

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 a pick

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

rem a pick

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

pkclear

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

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.

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

Show Amoeba

Display the masks used by the last INTEG command. Available only in 2D. Equivalent to the `SHOW AMOEBA` 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 curent 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 promt for parameters. There are general rules for parameter entering which I will try to descibe 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 theese.
- Some commands promt for spectral coordinates. Coordinates are always prompted as INDEX (this could be easily changed in the source, to pompt 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 finaly 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 combinaisons are meaningfull : 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 caracter. 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 centimeters.

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 PROCESSING

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

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

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 permits to share NMR files in a network, for instance a set of different workstations working with NFS on a file server. 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 ≤ 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.

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. 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 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.

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

These commands are for the basic Fourier transform step.

Depending on the spectrometer the data you get should 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!).

The 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
```

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......!?)

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 the 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 symetry of the phased line. A macro have been written which implements this method, it is called apsl, and works in 1D.

ADD, ADDH, ADDDATA, MULT, MULTDATA

Two data-sets 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.

Post processing : REAL, SWA, USWA, ABS, MODULUS, PLUS, MINUS, 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.

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 = $\sqrt{RR^2+RI^2+IR^2+II^2}$ 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.

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.

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.

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.

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.

SPECTRAL PARAMETERS

SPECW, OFFSET, UNIT, 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 (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), and SECOND(based on SPECW). All other values are invalid.

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. (used to be commands).

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

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.

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 nor displayed.

The scale is computed such that for SCALE=1, the larger point of the spectrum is full-screen. 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.

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 equal 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.

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.

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 <u>Zoom In</u> button (or on the display, with the left and right button of the mouse). Other controls in th ZM box are very natural.

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 appliy 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 strored 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

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. UNREF realizes just the inverse, i.e. display will not be refreshed, even if the previous commands did modify the data-set. UNREF is usefull in macro for fine control on the display. It is active only for the commands that preceedes 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

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 :

```
PEN : 1
      2
      3
      4
      5
      6
      7
      8
```

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.

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            ( VMS or UNIX)
```

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?, œ

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.

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).

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 ADDDATA

Is a generic buffer designed to be a “second hand”. It can hold 1D, 2D or 3D data-sets, accessed with GET and PUT, and can even be added to the current data-set with the ADDDATA command (single word).

FILTER, WINDOW

are two 1D buffers used to manipulate the current data-set. They are mostly designed to be used in conjunction with Maximum Entropy processing, but have some other use however.

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 very similar to FILTER as definition, but not as use. WINDOW is the description of valid points within the data-set (more precisely of \f(1;<σ>)). 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, etc… It is useful also to put to zero a certain region in a data set (for instance the water curtain in 3D).

Other buffers are available, used by the MaxEnt or the line-fitting package, see the specific documentations.

PUT, GET, SHOW, APPLY

are used to manipulate the different buffers.

PUT loads the given buffer with the current data-set

GET brings back the given buffer as the current data-set

SHOW displays the given information in the 1D window or in the 2D window

APPLY computes the result of the mathematical operation.

The buffer :	can be :	SHOW	GET	PUT	APPLY
WINDOW	window used to compute the chisquare in MaxEnt processing, also used by the polynomial mode of BCORR	•	•	•	•
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^{th} channel corresponds to the i^{th} 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.

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, see below.

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. Most of the commands works on all three modes, however, most of the commands will change their behaviour : for instance they will need more parameters.

Different commands

The following command will be strictly equivalent :

READL, READH, READV, WRITEL, WRITEH, ADD, ADDDATE, SIZE, LIST, ADDBASE, MULT, DSA, ABS, ONE, ZERO, PLUS, MINUS, ZM, PEAK, INTEG, LINEFIT

The following commands will now take more parameters instead of 1. In this case, in 2D the first one always refer to the F1 dimension (non-classical dimension, displayed vertically) and the second to the F2 dimension (classical dimension, displayed horizontally) ; in 3D the order will be F1, F2, F3.

CHSIZE, GB, LB, EM, GM, SPECW, OFFSET, EXTRACT, ZOOM, EVALN, SMOOTH, MEDIAN

The following commands will prompt you for an extra parameter which will describe which dimension the process should be applied : F1 means F1 dimension, F2 means F2 dimension, (in 3D F3 means F3 dimension) and whenever possible (noted (*) in the present list), combination F12 and F13 F23 F123 in 3D :

FT(*), IFT(*), RFT(*), IRFT(*), FTBIS(*), IFTBIS(*), PHASE, HPHASE, REVF(*), REVERSE(*), SIN(*), SQSIN(*), SWA(*),TM(*), USWA(*), BCORR

<u>*Commands more specific to 2D data-sets or 3D data-set*</u>

RZOOM (2D)

When in ZOOM mode, this command will jump to the symmetrical zoom window relative to the main diagonal of the spectrum.

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)

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

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.

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

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.

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 si_1_3d
   plane F1 $i plot *pl page *pl
endfor
```

would do the job.

You can also check the more developed macro : plot_plane_3d === distributed with the program.

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.

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 (since V3.0) 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 : •accessing the file from another program (may be another Gifa); •power failure of the computer; •a 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.

value of dim :	dimensionality of the JOINed file : 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 a little 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.

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 and proc3d

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.

<u>proc2d :</u>

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.

<u>proc3d :</u>

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.

UNDERSTANDING THE MEMORY SET-UP

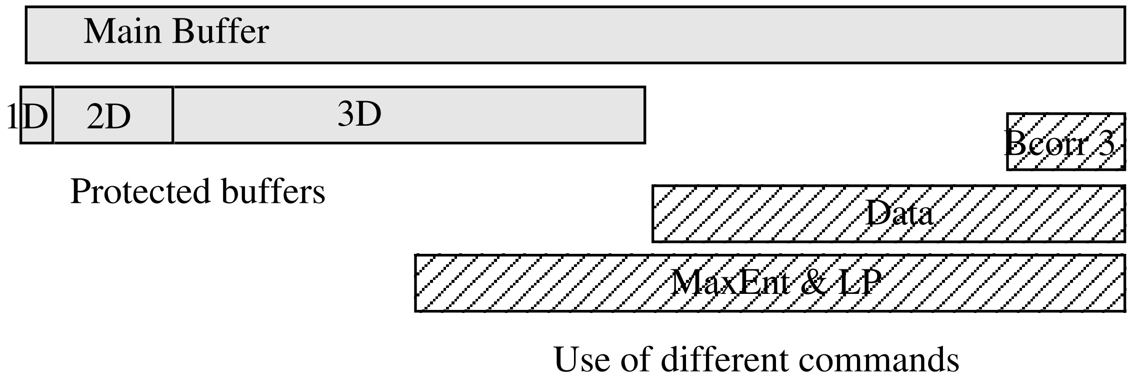
The Gifa program holds all the data in one single large memory buffer. This buffer is used for several purposes, and may be divided into smaller pieces. The size of this buffer is displayed when entering the program, or with the CONFIG command. There is no way to use a larger data-set than this memory 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 \f(1;2) of the size of the main buffer, the larger protected 2D is \f(1;4) of the larger 3D, and the protected 1D is \f(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 \f(3;4) of the main buffer so only \f(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 \f(1;8) of the main buffer. The PUT DATA and GET DATA command will use \f(1;2) of the main buffer. The BCOR 3 command will need only \f(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.

Gifa Memory Set-up :



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 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 linewidth; 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 developped 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 informations on the last peak 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. 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 pp has been designed to help in this process.

Viewing : 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*. Thus `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 with the CONNECT - DISCONNECT commands to generate listings.

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, PKCLEAR, PKCLEAN, PKRESET, POINT->PK, SETPEAK

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.

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 is another command for modifying the content of the peak table : the coordinates of a peak can be manually entered with this command.

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, MODIF_AMOEBA, mskread, mskwrite

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 three 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 define 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.

The amoeba can also be modified with the MODIFY_AMOEBA command which permits to set a given pixel to a given peak, or to remove it from the amoeba definition.

mskread and mskwrite are 2 macros meant for storing on file and retreiving the current peak and amoeba definitions.

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 : χ^2 = \f(1;n) \i\su(i;;\r(\f(\b(y_i-Y_i)^2;σ_i)))
Where Y is the recomputed spectrum, y is the current spectrum and σ is the variance of the noise, estimated from the NOISE command. Thus a correct fit corresponds to a final equal to 1.
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.
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.

SOMREC

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.

MORE SPECIFIC COMMANDS

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 visualizing 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.

PRINT, ALERT, MESSAGE

PRINT *text* will display the content of *text* to the user. ALERT *text* displays the text to user in a graphic box. ALERT will work whenever the graphic has been used once.

MESSAGE is used in macro, it is equivalent to PRINT, except that the string will be output to the user only if no parameters are available on the call line. It is thus nearly equivalent to

```
if (!$arg) PRINT text
```

However, it is different in the sense that the string will be presented in the graphic dialogue box when the macro is called from a menu button.

TEXT FILE INPUT / OUTPUT

Gifa has the capability of reading and writing on ASCII text files.

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.

OPEN CLOSE FPRINT <file_name eof(file_name)

It is also possible to read and write directly into text files. The command OPEN file_name, will open the file file_name for input or output. The command CLOSE will close the file. Ten different such files may be opened at once. An OPENed file may be written with the command FPRINT file_name output. A OPENed file may be read with the <file syntax (see below). When OPEN is issued on an already OPENed file, the file is rewound to the first line. The eof(file_name) function (see below) will have a value of 1 if the end of file was reached during the last <file_name operation and 0 otherwise.

Formatted output, the printf, fprintf, sprintf macros

There is no direct support for formatted output in Gifa, however, three macros have been written to implement this facility : printf, fprintf, abd sprintf. They are called by giving first a format, then a list of parameters (finished with a *). fprintf has an additive parameter which is the name of the file (which must have been OPENed first). sprint puts the result into a static variables called $returned.

eg :

```
printf "Size of the data-set \t%d x %d\n" $si1_2d $si2_2d *
```

These macros are implemented by calling 'awk' (a UNIX facility) with the SH command. This implies that : i) they are a bit slow; ii) they may fail (SH fails when the memory is low on the machine); iii) errors in formats will be detected by awk, not by Gifa (*nawk* has mush better error messages that the old *awk*); iv) type *man awk* to get information on the available formats.

SPECIAL AND GENERAL PURPOSE COMMANDS

HELP

permits to general info on a specific item. HELP with no arguments gives you the list of the commands available. (H or ? can also be used).

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.

^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, etc...

REF, UNREF

The 1D and 2D display are refreshed whenever the data are changed (or when a diaplay parameter has been changed (SCALE for instance)), REF and UNREF can force this behaviour. REF sets the internal Gifa flag, telling it to refresh the display, UNREF reset this flag such that no refresh will take place. However this flag is tested at the end of each command line, so REF and UNREF are usually the last commands.

SH, Unix calls

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

```
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

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.

SYNTAX OF THE GIFA INPUT.

Each command line is composed of a series of “words” separated by blanks. A word can be a command or a parameter. Words are strictly separated by blanks, however a word can be of several nature :

•literal are as typed:

```
chsize
```

•literal string are enclosed within single (') or double(") quotes:

```
'a string'  or "another string" or "yet an'other valid string"
```

•The special character `%` (to be used only as a parameter for a command) takes the place of the default value of the command:

```
EM %
```

•The special string `%%` takes the place of the whole series of all the default values of the remaining parameters of the command :

`ZOOM 1 % % % %` and `ZOOM 1 %%` are equivalent

Many commands know how to deal with this syntax, for instance BCOOR 1/2 needs a series of point to compute the baseline correction. If you have previously clicked on a set of points on the data, you will be prompted for the values corresponding to these points. So

```
bcorr 1 1 %%
```

will just do the work.

The baseline correction interactive macros use this feature.

•variables are substituted before use (more about this later):

```
$variable1
```

•expressions, enclosed within parentheses, are evaluated before use (more about this later) :

```
( 2*(cos(3) + 1))
```

•any of the preceding syntaxes may be preceded with a `<` symbol. In which case the input is interpreted as a file name, and the parameters takes the value of the next line read in the file (if already OPENed). A complete line is read at each time.

Each of these syntax can be used in any places; however, a single word cannot match a series of words :

These are valid syntax :

```
row $i                               ; select row i
row (%+1)                            ; select the next row
col (2*$i +1)                        ; select col 2i+1
set apod = 'sin'    $apod 0.5        ; perform sin 0.5
read ("/usr" // $user // $exp)       ; read a file
("simu" // "noe")                    ; execute the command SIMUNOE
set f = test open $f  row <$f        ; select the row whose index
                                     ; is found in file called test
```

These are invalid syntax :

```
set apod = 'sin 0.5'  $apod
```

a single word (here 'sin 0.5') cannot be used to match several words

```
    EM 1+2
```

the parenthesis are needed for expression to be evaluated
etc...

A line cannot be longer than 256 characters, otherwise the end the line will be lost. If a longer line is needed, a continuation sign is available : \
e.g.

```
Gifa>  print 'A line cannot be very long'     print \
\Gifa> 'But can be continued'   print 'as many time as you wish'
```

You can put as many continuation sign as you want, however, these signs are considered as “word”, so they should be blank separated, and cannot be used within evaluated expressions (see below).

VARIABLES

Variables can be used in Gifa, this feature is mainly useful when writing macro commands, however, it can be used at any time in the program. Variable are set (and created if not yet defined) with the command : SET :

```
Gifa> set b = 'hello world'   set c = 3
Gifa> set d := 'hello mom'              ; other syntax, see below
```

Variables are then just used by prefixing the name with a $:

```
Gifa> em $c    print $b
```

Variables can be used anywhere a regular entry is needed. Variables are not typed, but contain always a string. The maximum string is currently of 256 characters. The string is interpreted as a number when needed. Variable names are not case sensitive, the name is a maximum of 31 characters long; and must be built from purely alpha-numeric characters only (including the underscore : _). The number of available variables is limited at compile time (and reported by the command CONFIG, and variable $VAR_MAX (see below)), but a larger table can easily be built by recompilation if needed.

Associative arrays can be built using the construction [index] :

```
Gifa> set d[$k] = (cos($k/10))
```

Associative arrays means that each entry is created when needed, entries do not have to be sequential, and the index does not even have to be integer :

```
    $d[1] ; $d[3] ; $d[$z] ; $d['foo bar']
```

is a valid array. Associative arrays are coming from the standard UNIX program awk, search for a manual of this program if you some help with associative arrays. The function nextlm() permits to go through all the entries of a given array (see below).

Variables are allocated the first time they are set; referencing a variable not yet allocated generate an error. Variable are automatically deallocated when exiting the macro; they cannot be accessed by any other macros that would be executed during the life of the variable. In other words, variables have local scope, and are volatile (dynamically allocated and removed) (be careful, variables before v4.0 had always global scope !).

Variables created at interactive level (not within a macro) have a special treatment : their life will be as long as the program (unless an UNSET command is explicitly used), and they can be accessed by any other macro : they are static and have global scope.

If you which to create such a static variable from a macro (useful to remember parameters from one call to the other), you can use the following syntax :

```
    set d := 'this variable is static'
```

If `d` was already declared as volatile previously in the macro, the preceding command has the effect of creating a new variable, called d, but in the static storage, independent of the volatile d.

SET, UNSET, MUNSET, DUMP

The commands associated to variable handling are :

```
SET varname = value ; set (and create if needed) the variable
```

```
SET var2 = value    ; create and set a global variable
UNSET varname       ; remove the variable from the table
MUNSET list of vars finishing with a *
                    ; removes all the variables in the list.
DUMP                ; dump the content of all currently defined
                    ; variables
```

The format of the DUMP is : name of the variable ; context of the variable : (20 is static, 21 to 29 are macro call levels) ; content of the variable.

Using DUMP you will find that there might be entries in the variable table that do not correspond to user variables. This is due to the fact that the parser uses this table for particular use (dbm arrays, positions of label, location of WHILE, FOR controls). This entries have different formats from the user variables, thus cannot be mistaken with them. Some of these entries holds binary data that might disturb the terminal when using the DUMP command.

Internal variables

There are also special variables, not defined in the variable table, which takes the value of the internal parameters (contexts) of the Gifa program. These variables can be used, but should never be SET, they should be changed by using the associated commands. The list is currently :

```
$_             value of the next parameter present on the calling
               line. CANNOT BE USED WITHIN EVALUATED EXPRESSIONS.
```

if the following command is used :

```
@test 3 test.001
```

within the file test, $_ will be 3 the first time and test.001 the second time.
If no value is present on the calling line, the user will be prompted for the value

```
$ABSMAX        current value of ABSMAX
$ARG           True (1) if arguments are present on the calling line
               (within macro only)
$BUTTON        1,2 or 3 depending on which mouse button was last
               clicked
$CALIBDI[1]    the current calibrating distance, as defined with the
               CALIBDI command
$CALIBDI[2]    the current calibrating relaxation rate, as defined
               with the CALIBDI command
$CCOLOR        current value for CCOLOR
$CDISP2D       current value of command CDISP2D
$CHI2          value of the chi2 returned by the last command :
               MAXENT, LINEFIT, === RT->PK
$COL           index of the last extracted column in 2D
$COLOR         current value for COLOR
$CONFIG_GRAPH  is true if graphic is possible (X_window is
               connected)
$CONFIG_OS     The system type, as returned by the CONFIG command
$CONFIG_PLOT   The plot driver, as returned by the CONFIG command
$CONFIG_WIN    The window manager, as returned by the CONFIG command
$CX            current value for CX
$CY            current value for CY
$CZ            current value for CZ
$C_ABSMAX      value of ABSMAX of the currently JOINed dataset
$C_DIM         value of DIM of the currently JOINed dataset
$C_FREQ        value of FREQ of the currently JOINed dataset
```

$C_FREQ1	value of FREQ_1D of the currently JOINed dataset
$C_FREQ2	value of FREQ_2D of the currently JOINed dataset
$C_FREQ3	value of FREQ_3D of the currently JOINed dataset
$C_HEADER	last value accessed with the GETHEADER command
$C_JOINED	is if there is a currently JOINed dataset, 0 otherwise
$C_OFFSF1	value of OFFSET_1 of the currently JOINed dataset
$C_OFFSF2	value of OFFSET_2 of the currently JOINed dataset
$C_OFFSF3	value of OFFSET_3 of the currently JOINed dataset
$C_SIZEF1	value of SI1 of the currently JOINed dataset
$C_SIZEF2	value of SI2 of the currently JOINed dataset
$C_SIZEF3	value of SI3 of the currently JOINed dataset
$C_SPECWF1	value of SPECW_1 of the currently JOINed dataset
$C_SPECWF2	value of SPECW_2 of the currently JOINed dataset
$C_SPECWF3	value of SPECW_3 of the currently JOINed dataset
$C_TYPE	value of ITYPE of the currently JOINed dataset
$DIM	current value of DIM
$DISP1D	current value of command DISP1D
$DISP2D	current value of command DISP2D
$DISP3D	current value of command DISP3D
$DIST	the result of the last DIST command
$FREQ	main frequency (1H) of the spectrometer
$FREQ_1D	frequency in 1D
$FREQ_1_2D	frequency in 2D in F1
$FREQ_1_2D	frequency in 3D in F1
$FREQ_2_2D	frequency in 2D in F2
$FREQ_2_2D	frequency in 3D in F2
$FREQ_3_2D	frequency in 3D in F3
$GB1	value of gb in F1
$GB2	value of gb in F2
$GB3	value of gb in F3
$GIFAPATH	current PATH used for macro, set by th SETPATH command
$HOME	equivalent to the $HOME variable in UNIX
$ITYPE_1D	value of itype in 1D
$ITYPE_2D	value of itype in 2D
$ITYPE_3D	value of itype in 1D
$LB1	value of lb in F1
$LB2	value of lb in F2
$LB3	value of lb in F3
$LEVEL	current value of command LEVEL
$LICENCE	The licence as returned by the CONFIG command
$LOGA	current value of command LOGA
$MAX[1]	value of last computed max computed with the command MAX
$MAX[2]	value of last computed min computed with the command MAX
$MEM_MAX	The larger data set available, as returned by the CONFIG command
$MEM_PRO_1D	The size of the protected 1D area, as returned by the CONFIG command
$MEM_PRO_2D	The size of the protected 2D area, as returned by the CONFIG command
$MEM_PRO_3D	The size of the protected 3D area, as returned by the CONFIG command
$NAME	name of the current data-set
$NAR	number of A.R. coefficients as listed by ARLIST
$NOISE	value of the noise, as given by the NOISE command
$NPK1D	The number of entries in the 1D peak table
$NPK2D	The number of entries in the 2D peak table

```
$NPK3D         The number of entries in the 3D peak table
$NPOINT        The number of entries in the point stack
$NRT           Number of root as listed by RTLIST
$NSVD          Number of root as listed by SVDLIST
$OFFSET_1D     spectral offset in 1D
$OFFSET_1_2D   spectral offset in 2D in F1
$OFFSET_1_3D   spectral offset in 3D in F1
$OFFSET_2_2D   spectral offset in 2D in F2
$OFFSET_2_3D   spectral offset in 3D in F2
$OFFSET_3_3D   spectral offset in 3D in F3
$ORDER         current value for ORDER
$PH0           0th order of the last phase correction
$PH1           1st order of the last phase correction
$PK1D_A[i]     amplitude of the ith entry in the 1D peak table
$PK1D_F[i]     frequency of the ith entry in the 1D peak table
$PK1D_P[i]     phase of the ith entry in the 1D peak table
$PK1D_W[i]     width of the ith entry in the 1D peak table
$PK2D_A[i]     amplitude of the ith entry in the 2D peak table
$PK2D_F1F[i]   F1 frequency of the ith entry in the 2D peak table
$PK2D_F1W[i]   F1 width of the ith entry in the 2D peak table
$PK2D_F2F[i]   F2 frequency of the ith entry in the 2D peak table
$PK2D_F2W[i]   F2 width of the ith entry in the 2D peak table
$PK3D_A[i]     amplitude of the ith entry in the 3D peak table
$PK3D_F1F[i]   F1 frequency of the ith entry in the 3D peak table
$PK3D_F1W[i]   F1 width of the ith entry in the 3D peak table
$PK3D_F2F[i]   F2 frequency of the ith entry in the 3D peak table
$PK3D_F2W[i]   F2 width of the ith entry in the 3D peak table
$PK3D_F3F[i]   F3 frequency of the ith entry in the 3D peak table
$PK3D_F3W[i]   F3 width of the ith entry in the 3D peak table
$PKNAME        The name used by the last PKREAD / PKWRITE command
$PLANE[1]      axis of the last extracted plane in 3D
$PLANE[2]      index of the last extracted plane in 3D
$PLOTAXIS[1]   current value for the unit used in PLOTAXIS
$PLOTAXIS[2]   current value for the tick distance in x axis
$PLOTAXIS[3]   current value for the tick distance in y axis
$PLOTOFFSET[1] current value for plot offset on X axis
$PLOTOFFSET[2] current value for plot offset on Y axis
$POINTX[i]     X coordinates of ith point in the point stack
$POINTY[i]     Y coordinates of ith point in the point stack
```

coordinates are in index unit, absolute on the spectrum.

$POINTY[1] after a MONOPOINT in 1D, ranges between 0 and 1 depending of the position in the 1D window.

```
$RANDOM        a random variable in the range 0..1 with equiprobable
               distribution
$RANDOMG       a random variable with normal law, unit variance and
               zero mean
$RANDOMZ       same as $RANDOM but resets the random series
$RELAX         the result of the last RELAXRATE or SLOPE commands
$RCRYST        the result of the last RCRYST command CALIBDI
$ROW           index of the last extracted row in 2D
$SCALE         current value of the context SCALE
$SCOLOR        current value of the context SCOLOR
$SHIFT         value of the offset, as given by the SHIFT command
$SI1_1D        size of the 1D buffer.
$SI1_2D        size in F1 of the 2D buffer
$SI1_3D        size in F1 of the 3D buffer
$SI2_2D        size in F2 of the 2D buffer
$SI2_3D        size in F2 of the 3D buffer
```

$SI3_3D	size in F3 of the 3D buffer
$SIGN	current value of command SIGN
$SOMREC	value returned by the last SOMREC command
$SPECW_1D	spectral width in 1D
$SPECW_1_2D	spectral width in 2D in F1
$SPECW_1_3D	spectral width in 3D in F1
$SPECW_2_2D	spectral width in 2D in F2
$SPECW_2_3D	spectral width in 3D in F2
$SPECW_3_3D	spectral width in 3D in F3
$UNIT	current value for UNIT
$VAR_MAX	The total number of user variable available, as returned by the CONFIG command
$VERSION	The current version, as returned by the CONFIG command
$VHEIGHT	current value of command VHEIGHT
$ZOOM	1 if in ZOOM mode
$ZOOM_1D[1]	left coordinate of the 1D zoom window
$ZOOM_1D[2]	right coordinate of the 1D zoom window
$ZOOM_2D[1]	lower F1 coordinate of the 2D zoom window
$ZOOM_2D[2]	left F2 coordinate of the 2D zoom window
$ZOOM_2D[3]	upper F1 coordinate of the 2D zoom window
$ZOOM_2D[4]	right F2 coordinate of the 2D zoom window
$ZOOM_3D[1]	"left" F1 coordinate of the 3D zoom window
$ZOOM_3D[2]	"right" F1 coordinate of the 3D zoom window
$ZOOM_3D[3]	"left" F2 coordinate of the 3D zoom window
$ZOOM_3D[4]	"right" F2 coordinate of the 3D zoom window
$ZOOM_3D[5]	"left" F3 coordinate of the 3D zoom window
$ZOOM_3D[6]	"right" F3 coordinate of the 3D zoom window

SUPPORT FOR DATA-BASES

There is in Gifa a support for the UNIX standard data-base file format dbm. A dbm data-base is composed of two file : base_name.pag and base_name.dir which together hold the information of the base_name data-base. Each entry consist of a field indexed with an access key. Each entry is accessed with the access key. Data can be retrieve, stored, modified in the data-base. Every operations are realised on the file, but the disk accesses are minimised.

In Gifa, such a dbm data-base is accesses through a binding to an associative array. Each entry of the data-base appear as a element of the array. Reading, storing and modifying entries is performed by fetching and assigning array values. The access key of the entry in the dbm file appears as the index of the associative array, and the content appears as the value of the associative array. Due to internal Gifa limitation, only key up to 31 characters and entry up to 256 characters can be handled.

DBOPEN, DBCLOSE

These two commands permits to associate the dbm file with a pseudo internal array variable. The command

```
dbopen array_name file_name
```

will associate a pseudo associative array with the dbm files of base name : *file_name.* The file is created if it does not exist yet. No actual variable *array_name* is created, but each operation on it is performed on the dbm file.

DBCLOSE closes the file and forget about the array *array_name* .

The functions dbm() and nextlm() permits to handle the dbm file in macro processing.

EVALUATED EXPRESSIONS

Expressions can be evaluated in the Gifa program. Expressions should be enclosed in parentheses. Expressions can use most of the entries found in the paragraph SYNTAX, at the exception of the special entries : `%%` ; `<from_file` and the pseudo variable `$_` .

(2*(5-1)) (cos($i)) are examples of expressions. Expressions can be used whenever a Gifa input is needed (command as well as parameters). Expressions must fit on one line (i.e. 256 characters long), continuation mark cannot be used within expressions.

Values can be numeric, string or logical. Strings should be enclosed within '..' or "..". Logicals are stored as 0 for false and 1 for true (or any non-zero value).

Liste of functions and operators

The following operators and functions are implemented :

- the regular 4 operations : + - / * e.g. : (2*3 - 1)
- the modulo function : % (12 % 5)
- the power ^ operator (3^2.1)
- the regular mathematical functions : sqrt(x) cos(x) sin (x) atan(x) log(x) exp(x) abs(x) int(x) max(x,y) min(x,y)
- the special function power2(n) will have the value of the closest power of 2 below or equal to the number n : power2(130) will be 128 (=2^7)
- the concatenation operator : ('string1' // "string2")
- the formatting operator : ; equivalent to // ' ' //
  ("Value is:" ; $a) is equivalent to ("Value is:" ; // ' ' // $a)
- the alphanumeric operators : toupper(st) put string in upper case
  tolower(st) put string in lower case
  sp(i) generates a string of i blanks
  len(st) is the length of the string
  index(st1,st2) is the position of st2 located in st1, 0 if not present
  subst(st,i,j) is the substring from st, starting at i, ending at j
  head(st) will be the first word in string st (blank separated)
  tail(st) will be the string st but the first word.
  headx(st,c) and tailx(st,c) are equivalent to head and tail but the character c is used rather than blank.

- the numeral comparison operators : == != < > <= and >= for comparing numbers : ($x<=0.5)
- the string comparison s= (equal) and s! (different) for comparing strings : ($s s= 'name')
- the logical operators : | (or) and & (and) : (($x<=0.5)&($s s= 'name'))
- the not operation : ! : (!($i==1)) (!$arg)

• the function eof(file_name) will be true if the last input from file file_name (with <file_name>) had reached the end of the file, will be false otherwise.

• the function dbm(array_name) is true if array_name is bound to a dbm file with the DBOPEN command

• the function exist(var_name) will be true if var_name is a user variable either local or global. e.g.

```
if (exist("i")) set j = ($i+1)
```

j is computed only if $i exists as a variable.

The special syntax `(exist("foo[]"))` checks wheter the array foo exists with at least one index. It works both for regular and dbm arrays.

• the functions va1d(i), val2d(i,j) and val3d(i,j,k) returns the value of the content of the main Gifa working buffers. In 2D i and j are the index in F1 and F2 respectively, in 3D in F1, F2 and F3. This replaces the old $VAL[] construct.

• the function itoh(index,dim,axis), htoi(hertz,dim,axis), itop(index,dim,axis), ptoi(ppm,dim,axis), htop(hertz dim, axis) and ptoh(ppm,dim,axis) perform unit conversion. Respectively : index to hertz and back; index to ppm and back; hertz to ppm and back.

For each function, index, ppm or hertz is the value to be converted, dim is the dimension to use (1, 2 or 3) and axis is the axis to use, depending on which spectral widths and frequencies you want to use for the conversion.

• the next element function : nextlm. If i is an entry in the associative array $array, the construction nextlm(array,i) will have the value of the next available entry. The end of the array is notified with an empty string. The series is also initialised with an empty string. The series is gone through in the internal order which is not related neither to the input order nor the sequential order. For instance the following macro will print all the entries of the array $table :

```
set $index = (nextlm('table',' '))
while ($index s! ' ')
   print ($index // ' : ' // $table[$index])
   set $index = (nextlm('table',$index))
endwhile
```

Check also the macro tunset, which permits to remove all the entries of an array.

When evaluating expressions, all the internal computations are not typed and performed on strings. This permits to mix integer and string freely. Thus the following expressions are perfectly valid :

```
( cos(1) // 'a string' // ($i==1))
( toupper($file // ($i+1)) )
( log ('0.1') )
```

PROGRAMMING IN MACRO

Introduction to the control language

It is possible in the Gifa program to write command files (macros). The macro is then invoked by the command :

```
Gifa> @file_name
```

or simply

```
Gifa> file_name
```

In UNIX the macro name is the file name, sometime names with a .g extension are chosen (used to be .gif before the v4 version, but has been changed to separate from the popular graphic file format .gif). Any characters (but the blank) can be used in macro name, so ../test/my_macro or /usr/local/gifa/macro/startup.g are valid names.

A macro consists of a series of regular Gifa commands used as in the interactive mode. Up to 9 recursive calls may be nested (i.e. you can call a macro from within a macro, down to 9 nested levels). The macro execution can always be stopped with the ^C command.

Note that

```
Gifa> @file_name
```

The GifaPath

When calling a macro, the file first searched in the local working deirectory, and then is searched in a series of directories called the GifaPath. The default search order in the Gifapath is : the macro sub-directory of the home directory of the user (`$HOME/macro` in UNIX) and finally the standard directory : `/usr/local/gifa/macro` in UNIX. However the Gifapath can be modified at will (shortened or extended) with the SETPATH command. The current GifaPath can be examined with the $GIFAPATH context.

This is reminiscent with the notion of *path* in UNIX. This permits to build a library of macros, available for every Gifa user, as well as a set of commands personal to each user and to each project. The local directory is always searched first, so it is useless to add "." in the GifaPath.

The startup.g macro

When the Gifa program is first entered, it tries to execute the macro file called : startup.g, the file is searched in the GifaPath as any regular macro. Thus you can easily set-up you own environment. For instance your startup.g file (in your home directory, or in your working directory) may look like :

```
...any personal set-up
disp1d 1
/usr/local/gifa/macro/startup.g ; to be sure to have general set-up
```

You will find a comprehensive library of such macros in the /usr/local/gifa/macro sub-directory of the distribution kit.

The following commands are available for efficient command programming:

REFMACRO

REFMACRO (0 or 1)

depending on the value of this context, display will be refreshed at the end of each macro line (REFMACRO 1) as for regular processing; or only at the end of the macro execution (REFMACRO 0). Default value is 0; a value of 1 is useful only for interactive macros, or for debugging.

SETVAL, SETPEAK

SETVAL i {j { k } } val

will set the value of the ith point in the current buffer to val. The number of parameters for determining the point to be set depends on the value of DIM.

Similarly SETPEAK permits to change the coordinate of a peak table entry.

FOR, WHILE, IF, ERROR, GOTO

There are several control structures in the Gifa language. They are all pretty classical, and should not make you any problems.

```
FOR var_name = initial TO final { STEP step}
    .. some Gifa code
ENDFOR
```

This construction permits to write loops. The variable called *var_name*, will be created local to the macro if it does not yet exist, set to the value *initial*, and incremented by 1 for each loop. The increment can be different from 1 (but always numeric) with the optional field STEP *step*. *step* can even be negative, in which case the variable will be decremented. In any case, the test performed to determine whether the loop is finished or not is (*var_name* > *final*) if step is positive or (*var_name* < *final*) if step is negative.

```
WHILE some_value_to_be_evaluated
    .. some Gifa code
ENDWHILE
```

The Gifa code will executed as long as *some_value_to_be_evaluated* is true (is non zero). The value to be evaluated can be a variable or a complex evaluated expression into parentheses.

The IF command has two distinctive syntaxes : a one-line IF without possible nesting nor else; and a complete IF .. THEN construct with ELSIF and ELSE possibilities.

The multi-line IF is as follow :

```
IF test THEN
..commands on several lines
{ ELSIF test2 THEN
..commands }   (eventually many exclusive tests )
{ ELSE      (default case)
..commands }
ENDIF
```

The different commands will executed conditionally on the value of the tests. Any non-zero value is considered as true. If may be nested, with no limit on the number of nesting.

The one-line IF is as follow :

```
IF logical_value   ...remaining of the line ...
```

All the commands on the remaining of the command line are executed only if *logical_value* holds true (is non-zero).

examples :

```
IF ($X =< 0)  GOTO SKIP
print 'Hello' IF ($ITYPE_1D == 1)    set x = ($x+1)
IF (!eof(input)) print 'Still reading the file' \
                 set line = (%+1) \
                 IF ($line<$linemax) goto continue
```

tests to be used are described in the "evaluated expression" paragraph.

```
GOTO label
```

will redirect the execution of the macro to the symbol =label appearing somewhere else in the file.

Example

```
=loop
   ...any kind of processing...
   goto loop
```

GOTO should not be used to jump into FOR or WHILE loops, nor into IF .. THEN structures, Unpredictable execution will occur.

All these commands may freely nested. However, except for GOTO and the one-line IF, these commands (FOR, ENDFOR, WHILE, ENDWHILE, =label) should appear alone on one line, with no code preceding nor following the command (or the label), but eventually followed by a comment.

INITINPROGRESS, INPROGRESS

These 2 commands permits to build a bar showing the progress of the current command of the form :

```
In Progress : 0%....25%....50%....75%....100%
```

with a dot every 1/2Oth of the process

INITINPROGRESS tells Gifa how many iterations are to go, INPROGRESS actually does the display. INPROGRESS can be called at any rate, there is no need to do arithmetic to call INPROGRESS.

It is to note that, for a clean result, no terminal output should be performed during a INITINPROGRESS INPROGESS pair

Example :

```
set max = 1000
initinprogress $max
for i = 1 to $max
   ... do something
   inprogress $i
endfor
```

SETPATH, SETPROMPT

We have seen above that the SETPATH permits to modify the path used for searching macro files. There is also a SETPROMPT command, which permits to modify the prompt which is given to the user in the text window. Together with the macro and graphic capabilities, this permits to build easyly some applications, which does not even have to related with NMR. Some examples of this can be found in the contrib directory of the ftp server.

Interactive macros

During macro execution, it is possible to get input from the user in several ways :

• if a command misses a parameter, the user will be prompt for it, even if the macro is called deep in a nested loop. The user will be prompted with the current value. e.g.

```
    print 'Enter new size' chsize
```

(actually the message is not really needed, since the command CHSIZE will issue one)

If the macro is called from the graphic interface (with BUTTONBOX), either directly or indirectly called, a dialogue box will be used to prompt the user for the value, the message from the command (here chsize) will be in the dialogue box.

• by the same token, it is possible to assign the input into a variable :

```
    set b = 10   print 'Enter new value'  set b =
```

The user here will be prompted with the value 10 as default for b.

The command MESSAGE permits to put the message in the dialogue box if the macro is called from a menu button, and on the terminal if called from the prompt. Thus this is a better construct :

```
    set b = 10   message 'Enter new value'  set b =
```

• It is possible to get mouse coordinates with the MONOPOINT commands and the $POINTX[] and $POINTY[] variables. The ALERT command permits to build alert boxes, and BUTTONBOX and FORMBOX permit to build more sophisticate graphic interfaces.

Passing parameters to macros

Parameters can be sent to macros when called by following the call with the parameters to pass; within the macro file, these parameters will be obtain with the pseudo variable $_. each use of $_ "consume" one parameter on the call line. If no parameter is available on the calling line, the $_ pseudo variable will prompt the user directly. The variable $arg permits to test the presence of a value obtainable with $_.

For instance, if the file test_arg is as follow :

```
; to test argument passing
print $_
set b = $_   print (2*$b)
set c = $_
```

the following call

```
test_arg hello 3
```

will produce the following output

```
hello
6
```

and will prompt for the value to be applied to c. Thus $_ can be used to both the command line or the user, much in the same way as regular Gifa commands do. It is even possible to have an optional message, depending whether there is a parameter available or not, with the variable $arg :

```
if (!$arg) print 'Enter new value'
set b = $_
```

The MESSAGE command, has similar built-in mechanism, the string is sent to the user only if no parameters are available on the calling line. But it is better to use the MESSAGE command, since the message will then go to a dialogue box if the macro is called from the graphic interface.

```
message 'Enter new value'
set b = $_
```

Examples :

The PRINT command permits to output to the user a string. If you want to show more than a single line you can always use sh :

```
sh 'more text_file'           ; UNIX
```

As an example the 2D Fourier Transform could be written

```
; do the 2D FT in macro (specially silly),
if ($dim != 2) error 'Only in 2D'       ; do some checking
if ($itype_2d != 3) error 'Only on hypercomplex data-sets'
if ($si1_2d*$si2_2d) > 1024k  error 'too big for 4 times z-f'

print 'Processing in F2'
chsize % (2*power2(%))              ; zero-filling in F2
initinprogress $si1_2d      ; set up in progress bar
for i = 1 to $si1_2d      ; loop over rows
   row $i  dim 1          ; get ith row in 1D buffer
   ft                     ; process it
   dim 2  put row $i      ; put it back
   inprogress $i          ; display in progress bar
endfor

print 'Processing in F1'
chsize (2*power2(%)) %              ; zero-filling in F1
initinprogress $si2_2d
for i = 1 to $si2_2d      ; loop over cols
   col $i  dim 1          ; get ith col in 1D buffer
   ft                     ; process it
   dim 2  put col $i      ; put it back
   inprogress $i
endfor
exit
```

but don't try that one for real processing, it would be really slow!

A more useful example :

```
; do contour plotting in colours, 1 colour per level
; using scale, level and loga
if ($level>8) error 'Too many levels, should be <= 8'
```

```
set loc_lev = $level   level 1
set loc_sca = $scale
for i = 1 to $level
   pen $i %  plot %
   if ($loga!=1) scale (%/$loga)
   if ($loga==1) scale ( (%*$i) / ($i+1))
endfor
pen 1 % page %
scale $loc_sca    level $loc_lev
exit
```

Another example showing how you can build a special apodisation function in the window buffer and then use it :

```
; this macro builds a cosine roll-off apodisation function
; and applies it to the current data set
; works in 1D !
; in 2D, build the WINDOW only once and loop APPLY WINDOW on the 2D
put data                                 ; keep data aside
chsize (%/8) one sqsin 0
chsize (%*8) addbase 1  mult -1 reverse ; build apodisation
put window
get data    apply window                 ; apply apodisation
```

Here is a small (silly) interactive example :

```
; to compute the square root of a given number
sh 'more intro.txt'           ; some greeting message'
set i = 1      ;i should be set here for the following test to work!
while ($i <> 0)
   print 'Enter your number (0 to end)'
   set i = 0                  ; pre-set the value and ask for it
   set i =
   if ($i>0) then
         print ('Square root of';$i;'is';sqrt($i))
   elsif ($i<0) then
         print 'No real square root !'
   endif
endwhile
exit
```

For speed consideration it is always better, when working on a large macro, to make a small file for a very repetitive piece of work and call it. The looping as well as the parsing may get slow on a large file (typical on VMS systems). It is also slightly faster to call a macro with the @file syntax.

GRAPHIC USER INTERFACE

It is possible to modify and adapt the user interface within the Gifa program. The graphic user interface (GUI) is completely built from a simple set of basic commands which permits to build menus, dialogue boxes, etc...

BUTTONBOX, CLOSEBOX

The command BUTTONBOX creates a new entry in the menu bar, and create the menu bar for the first time. Parameters of the command are the name of the menu as it appears in the menu bar, then a list of entries consisting of the name of the button and the Gifa command associated to it. The lists end with a *. The special entry *separator* does not set a button but a separator in the box.

Any legal command can be used to be associated with a given button, a built-in command as well as a macro, and will be executed as if entered form the terminal. So the WHILE, FOR, IF .. THEN, GOTO commands are not available but the IF .. *any_command* syntax is valid. The action of the command in independent from the way it is called, except for the user prompting for values, which is performed with dialogue boxes in the case of a command called from a button.

Example given :

```
BUTTONBOX "my first menu" \
   Hello  "print 'Hello World'" \
   separator \
   Dim dim \
   "Test Dim" "if ($dim == 2) print 'We are in 2D'" \
   Back ("read" ; $name) \
   Reread  "read $name" \
   *
```

Which gives :

Note :

- How the command should on a single line, but how the continuation sign (\) can be used
- How the quotes are needed only to isolate field with blanks in it, for button names as well as commands (`Hello Dim`)
- How single and double quotes can be mixed to build composite commands (`Hello`)
- How the on-line IF can be used (`Test Dim`)
- How evaluated expression are evaluated when building the menu if not within quotes : `Back` reads the file which was last read when building the menu (the expression is evaluated when building the menu), `Reread` reads the file which is last read at the time the command is executed (`Back Reread`)

The command CLOSEBOX closes the menu bar and all the associated menus. It is equivalent to closing the menu bar from the close box.

MESSAGE

This command permits to build macros which have exactly the same behaviour than built-in commands. The macro `example`

```
message "Enter new size" set newsize := $_
```

will react as follow :

nothing will appear if called with a parameter :

```
example 256
```

the user will be prompted if called without parameters :
`example`
the user will be prompted in a dialogue box if the macro is called without parameters from a menu button.

In any case, this is independent of the way the macro is actually called, either directly or from within another macro.

FORMBOX, DIALOGBOX

These two commands are closely related.

DIALOGBOX permits to build sophisticated dialogue boxes, several fields can be built into the dialogue box, that the user has to fill-up. Each filed is internally associated to a Gifa variable, that the remain of the macro processes. The command appears as follow :

DIALOGBOX [series of entry] *

Each entry consists of a name, that appears as such in the dialogue box, and of a type for the field. Types can be : **message, string, int, real, file, enum**.

message type consists of a string that is displayed on the form and permits to put text in it.

The others type of field have two other entries which give the name of the associated variable and its default value. These types correspond to editable fields that the user has to fill-up. **string, int, real** correspond to string, real values or integer values respectively; **file** corresponds to a file-name entry, and presents a small additional button in the dialogue box, which permits to pop-up a standard Motif file selection box.

The last type : **enum** realises a pop-up menu, for an enumerated choice. It needs an additional entry which described the list of choice. Example given :

```
Dialogbox "my first dialogue" \
   "Enter below the file name to work on" message \
   "Enter file name" file var_file $name \
   separator \
   "Action to apply" enum "Read,Write" var_act % \
   *
$var_act $var_file
```

This macro will build a dialogue box with 2 editable entries : (filename and action) and will apply the action to the selected file if the user clicks on Ok.

Note :

- How the command should on a single line, but how the continuation sign (\) can be used
- The separator special field which builds a thin line in the dialogue box
- How the enumerated list is comma separated
- How the default value can be anything, here a Gifa internal variable ($name), and the default prompted value (%). In this last case, the default prompted value will be the value of the variable itself if the variable exists before the dialogue is built. If this is not the case, it will be the first entry for **enum**, 0 or **real** and **int** and the empty string for **string** and **file.**

• How the returned values are usual variables, and can be used for anything (here even as Gifa commands)

FORMBOX is the static version of DIALOGBOX. It builds a form that will remain after the completion of the command (as BUTTONBOX does) and will survive as long as the user does not explicitly closes it. FORMBOX needs an additional field (the callback) which describe the Gifa command to be executed when the user clicks on the Ok or Apply buttons. Apart from this, the definition of FORMBOX is strictly equivalent to that of DIALOGBOX. If not global, a variable associated to a field in a FORMBOX is local to the FORMBOX, and cannot be accessed in any other macros but the callback line. Example given :

```
Formbox "my first Form" \
    "print ('Hello';$y_name) print ('today it is';$the_wet) " \
    "Enter informations below" message \
    "Your name : " string y_name "unknown" \
    "The weather today :" \
    enum "Sunny,Rainy,Cold,Stormy,Terrible" the_wet % \
    *
```

Note :

• How the form variables can be used in the callback, in expression, as parameters for other commands

• Check other points in DIALOGBOX and BUTTONBOX

ERROR HANDLING

When an error is encountered, the program stops the execution and resumes to the user with a specific message. If the error happens during the execution of a string of commands on a single line, the string is aborted. If it happens during a macro, the macro is aborted.

Typical error conditions are :

• unknown command •wrong parameter for a command (e.g. FT F3 in 2D; SIN 1; FT on real data, etc..). • A impossible READx or WRITEx is tried (e.g. READ DATA.001 and DATA.001 does not exist). • mistyping a parameter (e.g. EM 0,5 instead of 0.5), • a ^C was typed by the user, • an ERROR command was issued.

If the error occurs when the command was executed from a menu button, a alert box will be displayed.

BATCH MODE

It is perfectly possible to create files in order to run the program in background.

On UNIX machines, type a file containing the command as you would type them and just start Gifa by "piping" the file as standard input, and the output on another file. The & sign run the process in background :

```
% gifa < name_of_the_COM_file > process.out &
```

Again, DO NOT forget the final EXIT. Also you may experience problems if you use interactive shell commands such as 'vi' or even 'more'.

On All Systems

The input in the batch file is entered to the program as a user would do, so it is different from macro (of course not for macros called during the batch) in at least to points : •control structures are not allowed •error conditions will not stop the execution, but the program will continue, So be careful when deleting important files within batch files!

When running in batch mode it is usually useless (though not forbidden) to activate the display. However if you want to have Gifa running while you are not logged on, you should choose a graphic-less mode. This mode is entered if there is no X_window DISPLAY available. For instance with

```
unsetenv DISPLAY
```

Do not forget to adapt a special startup.g macro (for instance in the current disrectory) in order not to launch the standard graphic environment (which would give an error anyway).

It is perfectly possible to plot and print results while in batch mode.

FREQUENTLY ASKED QUESTIONS

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

Due to my laziness, The reference for the Gifa program is only submitted. Currently, the first and only reference of a paper completely devoted to Gifa is :

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

Pons, J.L., Malliavin, T.E. and Delsuc, M.A., submitted. Gifa V4 : a complete package for NMR data-set processing.

which will describe Gifa (if ever accepted)

You may also use the following references :

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

for the J-Deconvolution method

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

for the Hyper Complex Fourier transform

Application of Maximum Entropy Methods to NMR Spectra of Proteins. M.A.Delsuc, M.Robin, C.Van Heijnoort, C.B.Reisdorf, E.Guittet and J.Y.Lallemand. NATO WorkShop Il Ciocco. (1990)

generic text on use of MaxEnt

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

MaxEnt in 3D

"Compression of Multi-dimensionnal NMR Data-sets" Thérèse E.Malliavin, Marc A.Delsuc, Jean-Y.Lallemand, *J.Magn.Reson.* **94** p 630-634 (1991)

the READZ WRITEZ commands

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

the SMOOTH command

“Le traitement des données en RMN” M.A.Delsuc, P.L.Fortier, C. van Heijenoort, T.Malliavin, M.Robin, A.Rouh, *les Cahiers IMABIO* **3** p49-61 (1992)

generic text on use of MaxEnt

“Computation of Redfield Matrix Element from Incomplete NOESY data-sets” Thérèse E.Malliavin, Marc A. Delsuc and Jean Y.Lallemand. *J.Bio.NMR.* **2** p 349-360 (1992)

the Build-up curve processing part

“Accurate estimation of inter-atomic distances in large proteins by NMR” Christine Reisdorf, Thérèse .Malliavin et Marc A.Delsuc; *Biochimie* **74** p809-813 (1992)

another reference

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

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 (mad@cbs.univ-montp1.fr) I will send you the licence agreement. Relax, the licence of Gifa is free for academic labs.

Q : I get the message - startup.g : command unknown - ?

then Gifa runs correctly, without the graphical environment.

The installation is not complete. To work correctly, Gifa needs a set of directories and file which should in /usr/local/gifa . Usually this is done by using the installation procedure distributed with the program, which sets a link (ln -s) between the location where Gifa actually is and this standard address.

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

then Gifa stops on error during the start-up procedure.

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 : 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 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 :

o 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.

o the disk is full, or your quota is exhausted

o 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 : 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

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 command. Use the WRITET 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 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 imaghinary parts; etc... etc...

There are many possibilities in Gifa, try to play with FT RFT FTBIS; REVF INVF; SWA USWA. Once you have found a set-up, you might want to propagate it in the macros ft_* found in the distribution.

Q : I processed Bruker-DMX data-sets, what is going on ?

The DMX machines, equipped with a digital filter, do not store the FID in its genuine acquisition format, but after a first processing which is done on-the-fly during the acquisition. This processing appears to be "non-causal", i.e. there non-zero data-points before the actual initial time t=0 of the acquisition. These points are stored by Bruker at the beginning of the file and are usually of the order of ~140 (but it is not constant and seems to be related to the acquisition parameter DECIM). There are actually several ways of processing such data-sets.

- throw those points awy with a lshift (leads to not-so-nice baselines)

- append this non-causal part at the end of the FID (a bit complicated to do)
- process as usal and then apply a ~25000 degrees first order phase correction. Formally equivalent to the former, but much simpler to do.

There is a complete discution of this problem at : gopher://gopher.nmrfam.wisc.edu/00/digfilt2 due to W. M. Westler and F. Abildgaard.

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 : How can I start Gifa in background job ?

See documentation above.

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 variable 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 nternal 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).

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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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