
Chapter 5

Pulse program display

The command “*Utilities/Show pulse program*” in main NMR-Sim menu opens a new window, which shows the selected pulse program in a graphical form.

The pulse programs are shown in a symbolic form, i.e. the lengths of pulses and delays do not represent the actual durations, but they use a artificial proportions which make the pulse program more understandable.

The pulse program display may be also started as a stand-alone application:

nmrsim -showp <pulse program name>

This command opens a pulse program display window without any simulation functions. There is possible to start any number of copies of the stand-alone display (The NMR-SIM program may be started for each user only once).

Equivalent command is also available direct from TOPSPIN:

spdisp <pulse program name>

displays the pulse program

spdisp

reads the pulse program name from the current data set.

You may also switch to the pulse program tab in the TOPSPIN data set window and

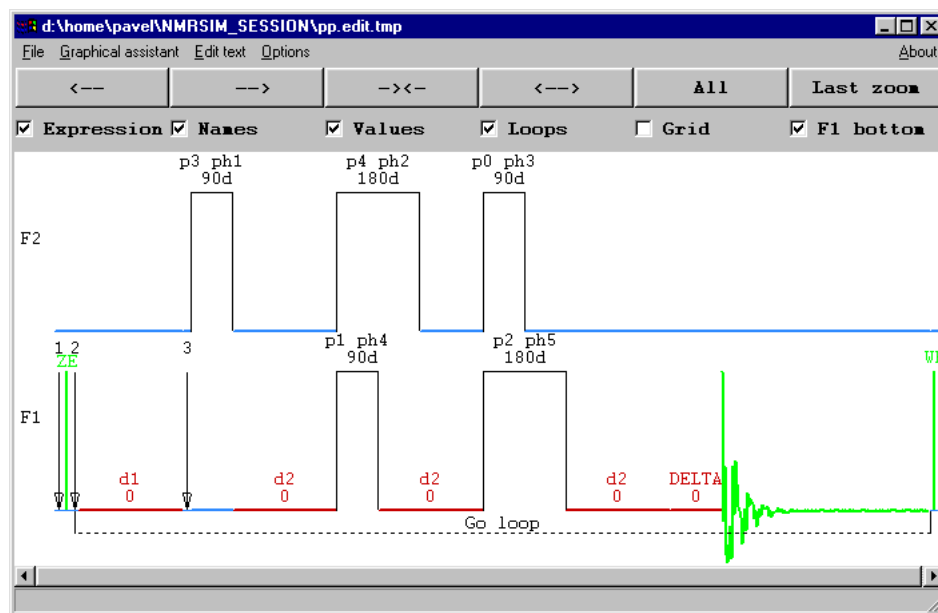


Figure 5.1 Window with the pulse program scheme

press the graphical pulse program display button (Figure 5.2).

The menu bar in the stand-alone version contains two additional commands: *Graphical assistant* and *Edit text* (see “Graphical assistant for pulse program editing” on page 75 and “Pulse program text editor” on page 84)

The buttons on the top of the pulse program window and the scroll bar on the bottom can be used to zoom and scroll the pulse program display.

You may also zoom using the mouse. The procedure is the same as zooming in TOPSPIN: press the left mouse button on the start of zoomed area and drag the mouse to the end. The expanded area is highlighted by two vertical cursor lines and middle thick line:

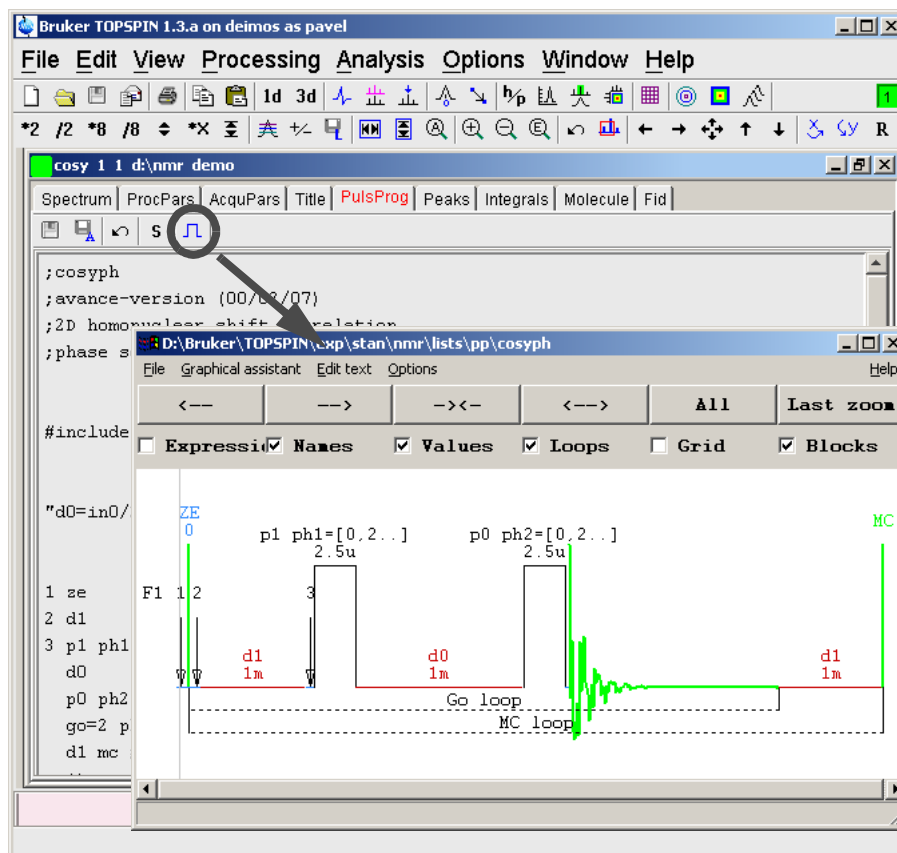
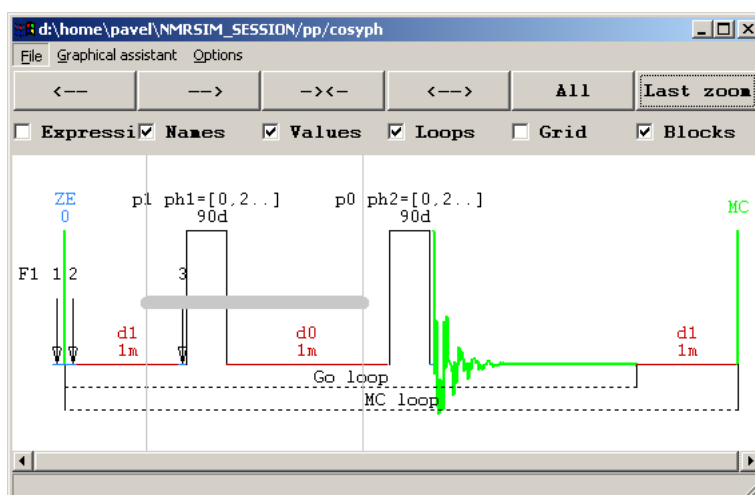


Figure 5.2 Pulse program display from TOPSPIN PulseProg table.



Releasing the left mouse button displays the selected part of pulse program.

The button "<-->" zooms in to the pulse program (shows more details), pressing "--><" zooms out. The command *All* shows the whole pulse program again, *Last zoom* brings back the last expansion.

5.1 File menu

- **Select**
Select a new pulse program to be displayed. This will not affect the pulse program selection in the main NMR-SIM window. The selection uses the TOPSPIN *edpul* dialog for the selection of pulse programs from the data base.
- **Page setup**
the page setup dialog defines basic parameters for printing. You may select the size of the printout, the size of used font and switch on/off the colors.
- **Print**
Print the pulse program scheme on the current printer.
- **Copy to clipboard**
Copy the picture in the MS-WINDOWS metafile format to the clipboard. This allows easy transfer of pulse program schemes to other programs.

Windows

- **Movie**
This command shows all available pulse programs from the pulse program database in series.
- **Close**
Close the pulse program display window and pop-up the main NMR-SIM window.

5.1.1 Using “Drag and Drop” for the file selection

Drag and drop provides a very efficient mechanism for the enhancement of the user interface. The pulse program display uses the *drag and drop* mechanism for the selection of the pulse program being displayed. This method works only for older pulseprograms which are not yet stored in the database (Figure 5.3)

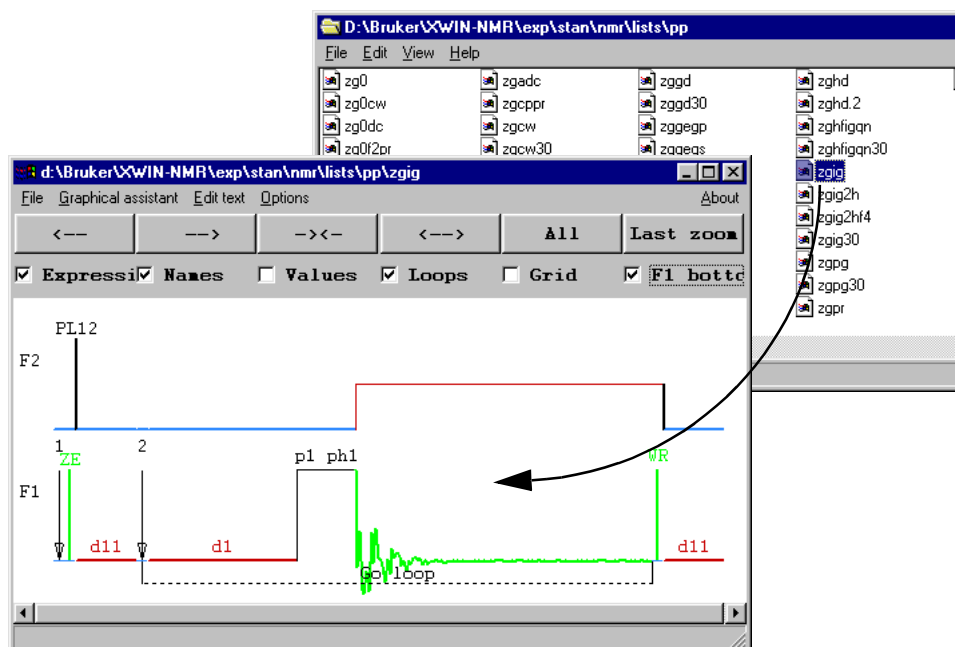


Figure 5.3 Pulse program display window with the MS-WINDOWS explorer window in background. The explorer window shows all available pulse programs. Use drag and drop to visualize the pulse programs.

5.2 Options menu

The *Options* menu controls the features of the pulse program display.

5.2.1 Display

The *Display* command opens a dialog box used for setting the following parameters:

- ***Pulse program selection path***
Selects if the pulse program selection dialog uses as starting directory the default path, or the path where the currently shown pulse program resides. This option is used only if you select pulse programs from disk.
- ***Background***
Here you can select the background color. The colors used for the pulse program display are changed automatically to get a optimal contrast for all elements.
- ***Pulse height***
Controls how the pulse program display shows the pulse height
Constant - all pulses have the same height
Proportional to power level - the program uses following formula to calculate the pulse height


```
if (powerLevel < 20 dB)
    height = exp(-(powerLevel+6)*0.0266595);
else
    height = 0.7598*exp(-(powerLevel+6)*0.0160944);
```
- ***Show disk commands***
Toggle the display of disk commands (*wr*, *if*). The disk commands are marked as vertical marks in the pulse program diagram.
- ***Show loops***
Toggle the display of loops and labels in the pulse program. The loops are marked as dashed lines below the acquisition channel, the symbol used for the label is a vertical arrow with the label on the top.
- ***Names***
Toggle the display of pulse and delay names.

- **Parameter Values**
Toggle the display of parameter values (see “Event names and parameter values” on page 86).
- **Grid**
Switch the grid lines in the pulse program display. The grid lines between different channels connect synchronous points in the pulse program. This is an important feature for the visualization of “pulse trains”. A pulse train is a parallel asynchronous execution of pulses and delays in two or more channels (see “Synchronization of events - grid” on page 90).
- **Evaluate expressions**
This switch controls the evaluation of expressions in pulse program (see “Expressions in pulse programs” on page 90).
- **Evaluate compiled if {}**
Defines if the pulse program display shows all branches of “*compiled if*” expressions, or if the test expression is evaluated and only currently active parts are visible.
- **Show 3D gradients**
Selects if the all three (x,y,z) gradient components are visible. Pulse programs using the imaging gradients (*grad {..}*) show always all three components.
- **Show real waveforms**
Controls if the pulse program display reads and displays the actual waveforms stored in the parameters, or uses symbolic shapes.
- **Show phase values**
Check it, if you would like to see the phase values for each pulse. The pulse program display shows all phases for short phase tables, or only the start of the table for long ones.
- **Show nuclear labels**
Selects if the pulse program display shows corresponding nuclear labels instead of channel names
- **Display Event channel**
Select if the event channel is shown. The event channel shows several spectrometer controlling events as DWL_CLCK_ON. Most of these events are in fact pulse program macros using the *setnmr* control command.
- **Display channels without active commands**
You may hide here the display of channels containing only delays.

- **Channels** - select the arrangement of the spectrometer channels on the display. You may place the acquisition channel either on the top, or on the bottom of the pulse program display:

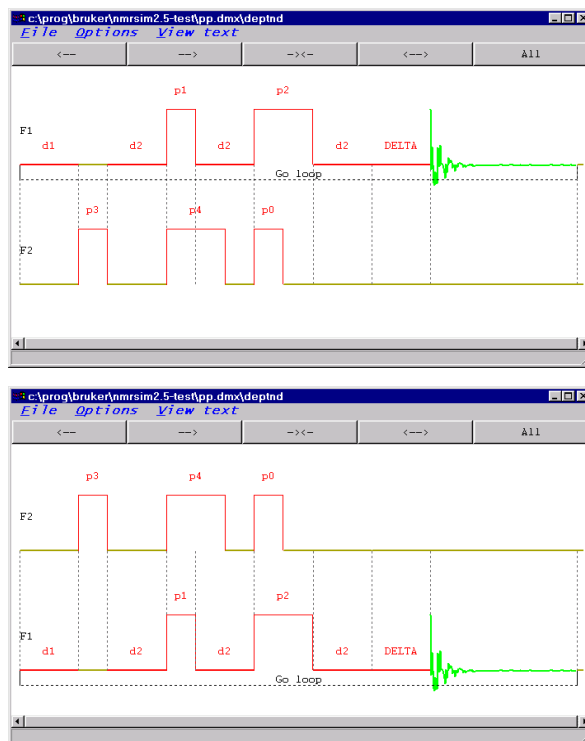


Figure 5.4 Different channel arrangement in the pulse program display

Several of these settings are also available in the tool bar on the top of the pulse program window.

5.2.2 Configuration

The commands *Configure pulses* and *Configure delays* allow you to set the relative width and height of the pulse box, or the length of the delay on the display. The Figure 5.5 presents two possible layouts of the *DEPT* pulse program.

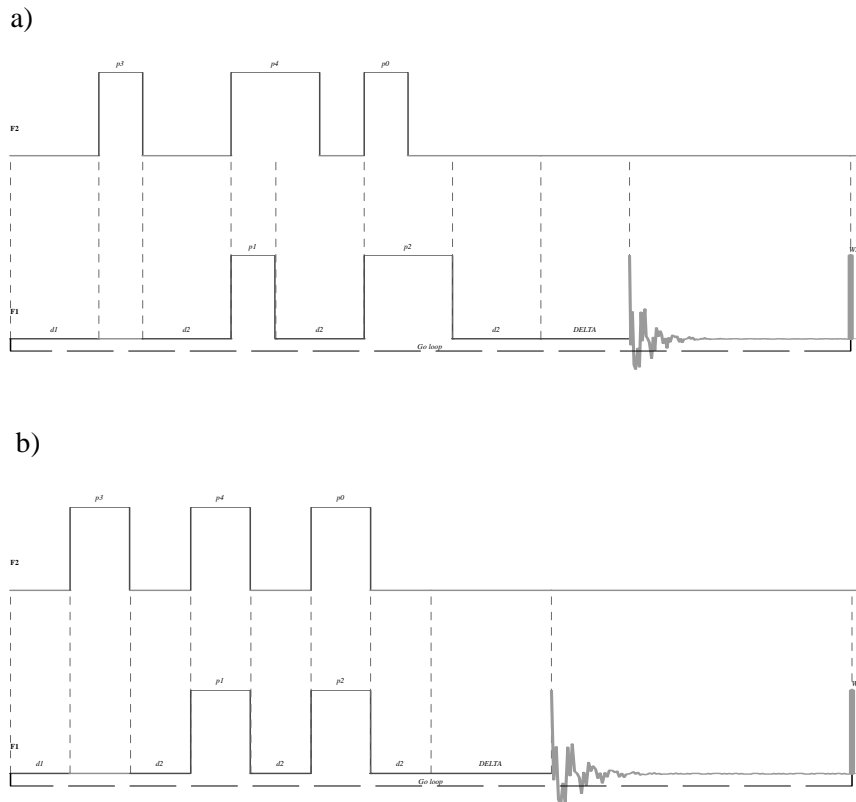


Figure 5.5 DEPT pulse program with two different pulse and delay configurations. The picture a) uses different pulse width to visualize different pulse length (this is the default layout. The picture b) uses the same width for all pulses.

The configuration may be stored to disk (commands *Load configuration* and *Save configuration*).

The *Restore defaults* command restores the original pulse program display configuration.

5.2.3 Fonts

Windows

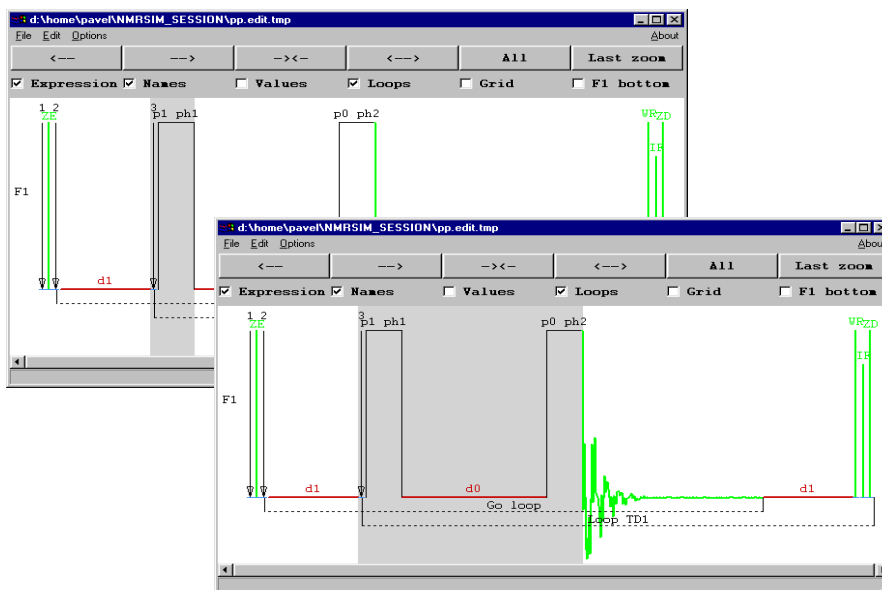
The fonts menu allows to set the font family and the font resizing policy for the pulse program display window. More details are available in the section ***Font selection*** on the page 169 in Appendix.

5.3 Graphical assistant for pulse program editing

Writing of pulse programs may be very tedious tasks for people which are not familiar with the details of the pulse programming language. The *Graphical assistant* allows you to write your own pulse programs, or modify the existing ones without the necessity to learn the pulse programming language. The graphical assistant creates always Avance series compatible pulse programs. The AMX family of spectrometers is not supported.

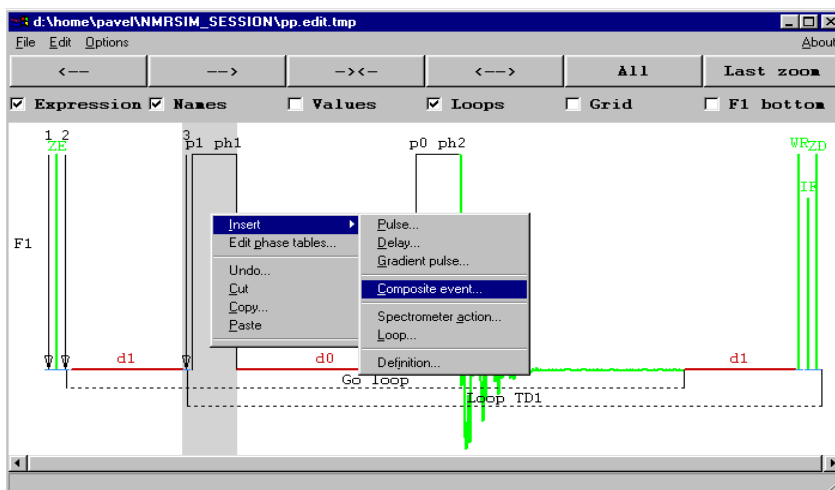
You edit the graphical representation of the pulse program in a similar way as you would edit the text, but you handle whole NMR objects and not their text description. You may copy, cut and paste objects, you have a undo function.

Clicking the mouse in the pulse program graph highlights one pulse program element. Pressing the Shift key on the keyboard allows you to select a region between the old selection and the new cursor position:



The selected element defines a reference position (cursor position) for editing commands. All the editing commands are either available from the pull-down menu *Edit*, or from the context sensitive popup menu, which is activated when

pressing the right mouse button:



Each item in the *Insert* menu allows you to insert one class of NMR experiment events. Each class of NMR objects has its own dialog defining the basic parameters and features.

5.3.1 Pulse, delay, gradient pulse

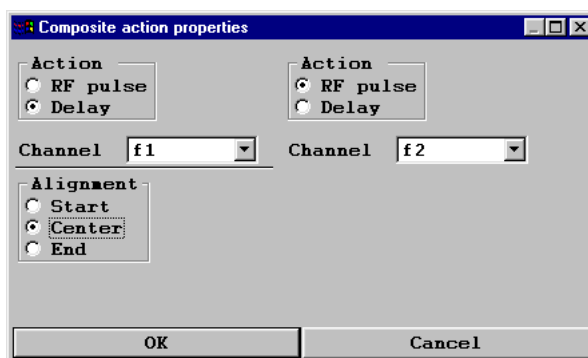
Menu items *Pulse*, *Delay* and *Gradient pulse* enter one specific event.

The names of these standard objects, as “*High power 90 deg pulse*” and their mappings to pulse program parameters as “*p1*” are the same as the names and mappings used in all standard Bruker pulse programs and described in the file *Param.info* in the pulse program directory.

5.3.2 Composite event

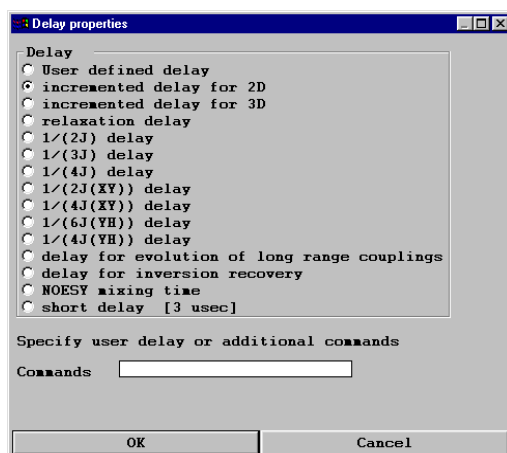
Composite event denotes a combination of two pulses or delays in one or more channels (pulse train). You may define the type of the action for each channel, the

channel and the required alignment of events.



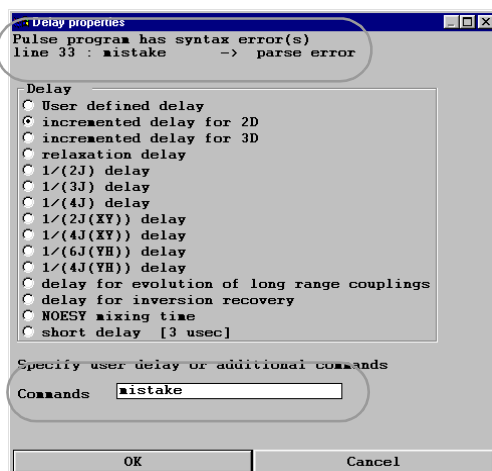
The graphical assistant asks you for the property of each action. The names of the actions and the corresponding parameters (pulse, or delay) are the same as the standard used for the Avance Bruker pulse programs.

The Delay properties dialog defines the type of the delay. You may also specify additional commands or spectrometer switches in the line *Commands*. The graphical assistant checks the syntax of your additional input.



In the case of errors in your input, the input dialog appears again and the correction

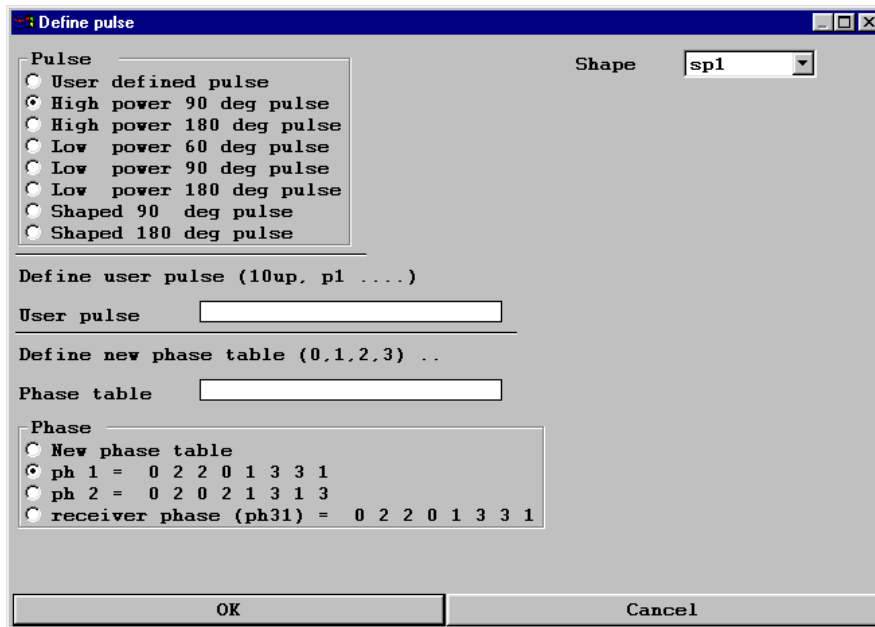
of the input is required:



However, the input correction may be required only for your input. The commands entered in the pulse program by the graphical assistant is always correct.

The dialog defining the features of radio frequency pulse is similar to the delay dialog. There are additional fields for the selection of channel, phase and the optional shape function for shaped pulses. You may either select one already exist-

ing phase table, or define a new one.



The marked parts of the text show the text representation of one composite object defined in previous steps. The graphical assistant supposes always, that the delay

is longer than the pulse.

The screenshot shows a pulse program editor window titled "d:\home\pavel\NMRSIM_SESSION\pp.edit.tmp". The main window displays a timing diagram with two pulses, F1 and F2. Pulse F1 is shown in green and pulse F2 in blue. Delays d1 and d2 are indicated by red lines. A calculated delay CEN_D01 is shown in blue below the pulses. The code in the right-hand pane defines CEN_D01 as $(d2 - p3) / 2$.

```

File
782 bytes saved to d:\home\pavel\NMRSIM_SESSION\pp.edit.tmp

#include <Avance.incl>

::"d0=3u"
3m ; do not delete this delay

define delay CEN_D01
"CEN_D01 = ( d2 - p3 ) / 2 "

1 ze
2 d1
(d2 ):f1 (CEN_D01 p3 ph1):f2
3 p1 ph1
d0
p0 ph2
go=2 ph31

```

Entering two parallel pulses creates more complicated situation. The code entered in the pulse program defines two additional delays and calculates their values so, that the pulses will be always centered. Independent on the relative length of both pulses.

The screenshot displays a graphical assistant for pulse program editing. The interface is divided into two main sections: a graphical waveform editor on the left and a code editor on the right.

Graphical Waveform Editor:

- F1:** Shows a red horizontal line representing a pulse. It starts with a delay of $3m$ (3 milliseconds), followed by a pulse of duration $d1$. A green vertical line labeled ZE is positioned at the start of the pulse. A vertical line labeled $p1$ is at the end of the pulse.
- F2:** Shows a blue horizontal line representing a pulse. It starts with a delay of CEN_D02 , followed by a pulse of duration $p3$ and phase $ph1$.
- F3:** Shows a blue horizontal line representing a pulse. It starts with a delay of $p22$, followed by a pulse of duration $ph2$.

Code Editor:

The code editor shows the following code:

```

define delay CEN_D02
define delay CEN_D12
if " p3 <= p22"
{
"CEN_D02 = ( p22 - p3 ) /2 "
"CEN_D12 = 0"
}
if " p3 > p22"
{
"CEN_D12 = ( p3 - p22 ) /2 "
"CEN_D02 = 0"
}
1 ze
2 d1
(CEN_D02 p3 ph1):f2 (CEN_D12 p22 ph2):f3
3 p1-ph1

```

A message box indicates "939 bytes saved to d:\home\pavel\NMRSIM_SESSION". The code editor also shows "line 29" at the bottom.

5.3.3 Spectrometer events

The menu item *Spectrometer event* may be used to enter special events like Decoupling switch, or gradient block/unblock commands. All spectrometer events include some short delay necessary for the spectrometer hardware to execute the command.

The spectrometer events include also the decoupler settings and power level changes.

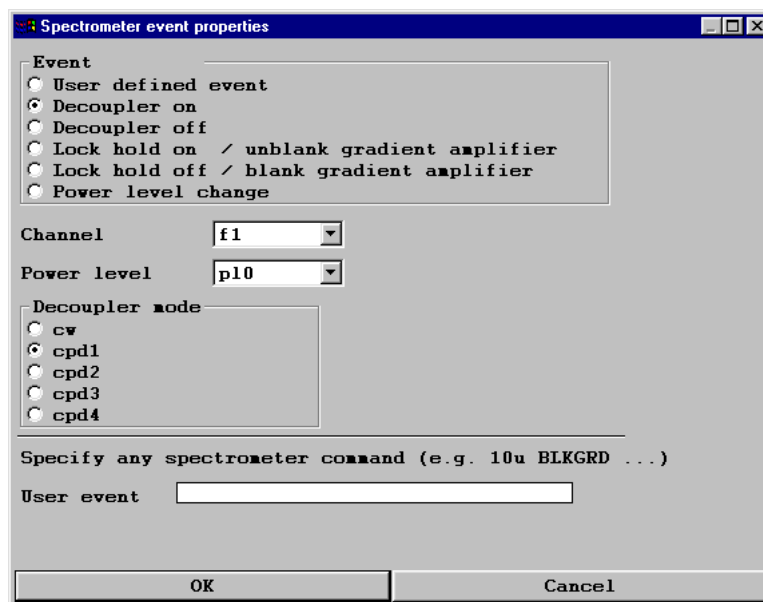
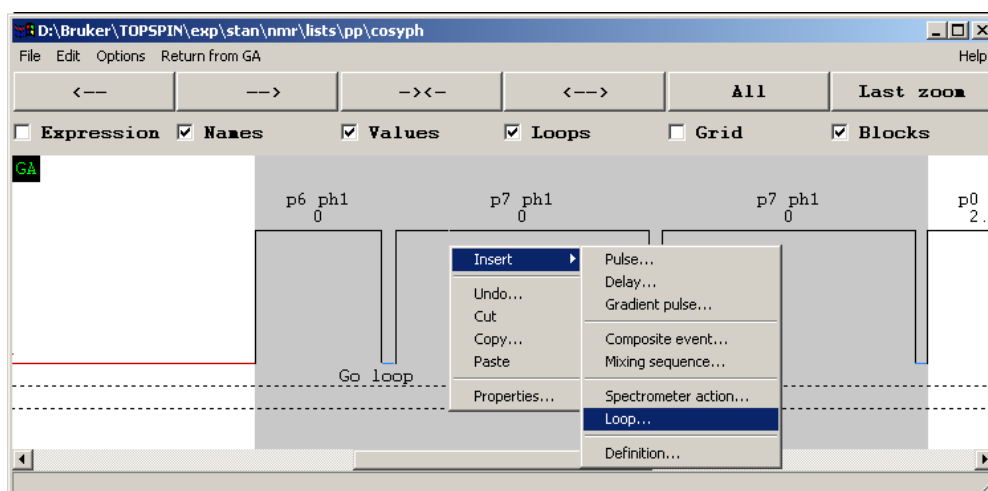


Figure 5.6 The Spectrometer event properties dialog

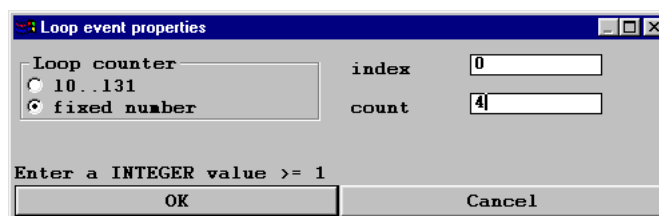
5.3.4 Loops

The *Loop* command is used to enter a pulse program loop.

Select the region in the pulse program, you would like to repeat. Press the right mouse button to get the context sensitive menu and select the item "*Insert/Loop*":



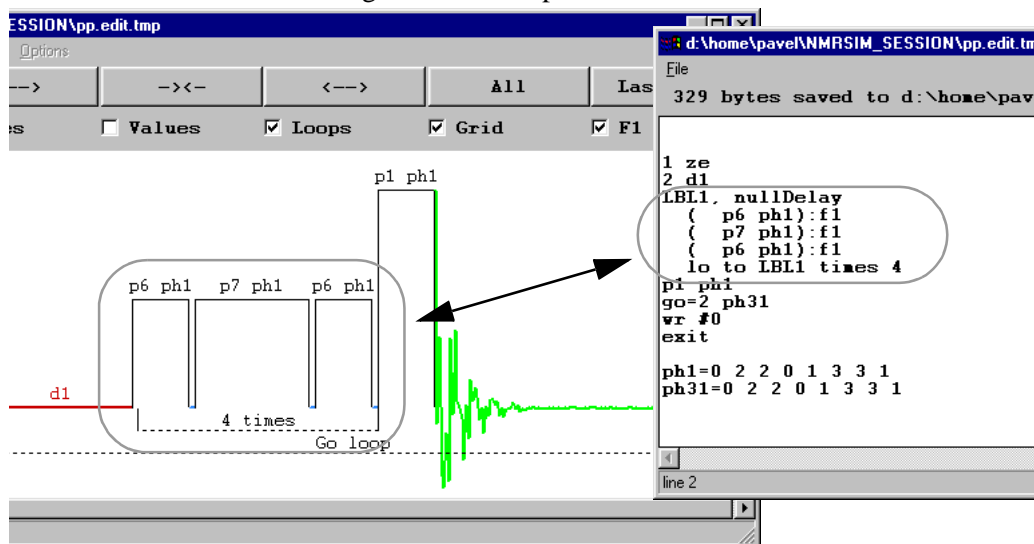
The loop counter is defined either as a loop variable *10..131*, or fixed integer num-



ber.

The Graphical assistant generates for each loop a new labels in the form “*LBL<number>*”. A dummy delay *nullDelay* is used as the “placeholder” for the label. The length of this dummy delay is set at the start of the pulse program to

zero and so it will be ignored on the spectrometer hardware.



5.3.5 Definitions

The command definitions allows you to enter a definition of user defined pulse, delay, or list.

5.4 Pulse program text editor

The NMR-SIM program offers the possibility to couple the pulse program text editor to the pulse program display. This feature may be switched on or off in the *NMR-SIM Options* dialog. See “Options” on page 32.

The pulse program display is updated after each change of the pulse program. It is possible, that the actual version contains a syntax error. In such a case the pulse program display shows the last syntactically correct version and the message line of the display window displays the error message.

The cursor position in the pulse program text is highlighted in the pulse program diagram as a region with a different background color. This feature simplifies the orientation in complex pulse programs.

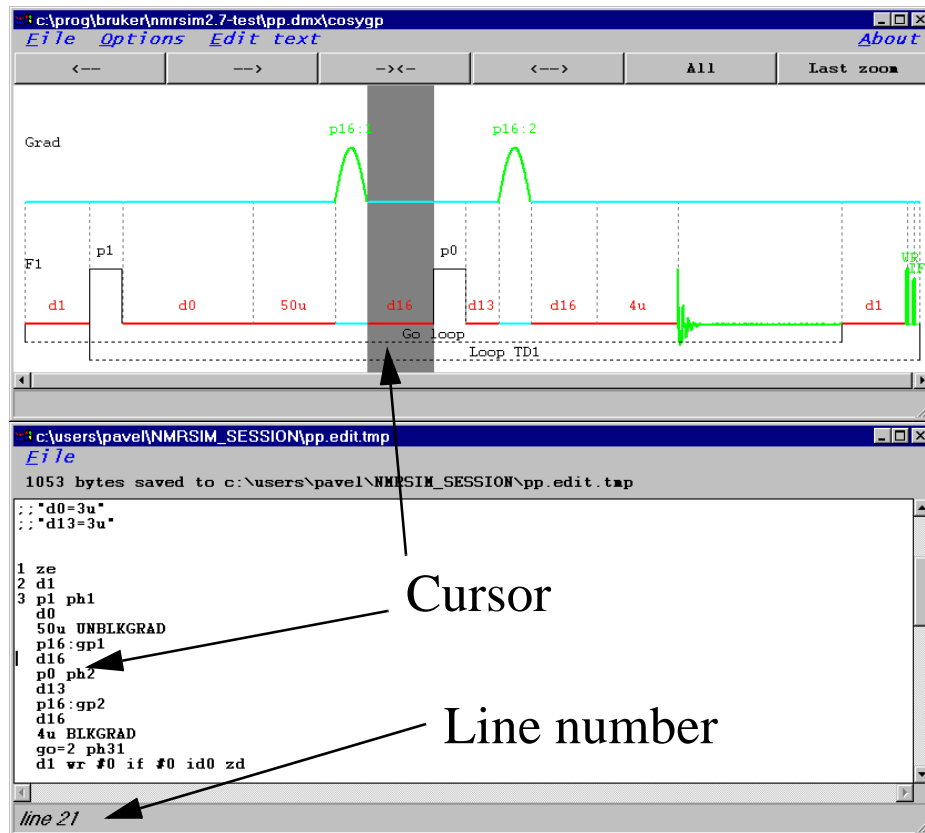


Figure 5.7 Pulse program editor. The cursor position in the text window is highlighted on the pulse program display

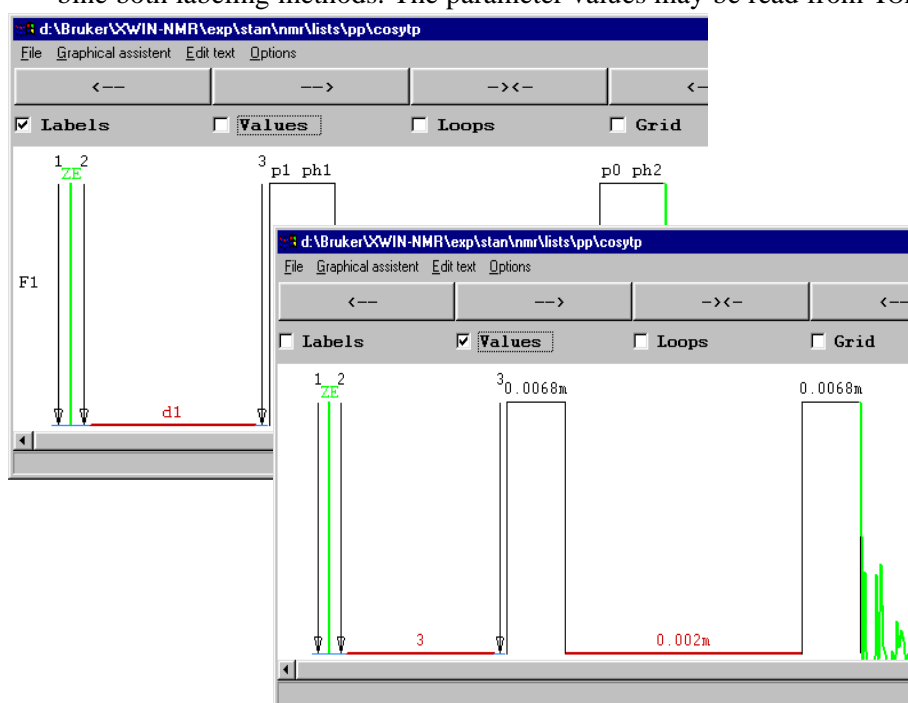
5.5 Pulse program visualization details

5.5.1 Spectrometer channels

The pulse programs use spectrometer conform labels $F1..F8$ and $Grad$ for gradient channel. the switch “***F1 bottom***” defines the position of the $F1$ channel: either on the top, or on the bottom of display.

5.5.2 Event names and parameter values

The pulse program events may be labeled using their names (e.g. $p1$, $d1$) or using the actual values of their respective parameters. Following picture shows a part of COSY pulse program with labels and parameter values. It is also possible to combine both labeling methods. The parameter values may be read from TOPSPIN data

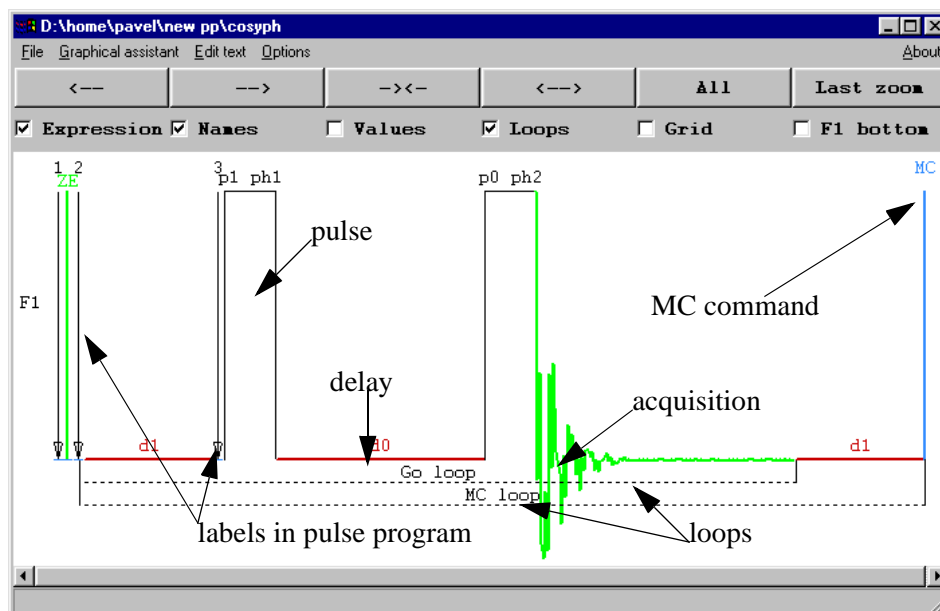


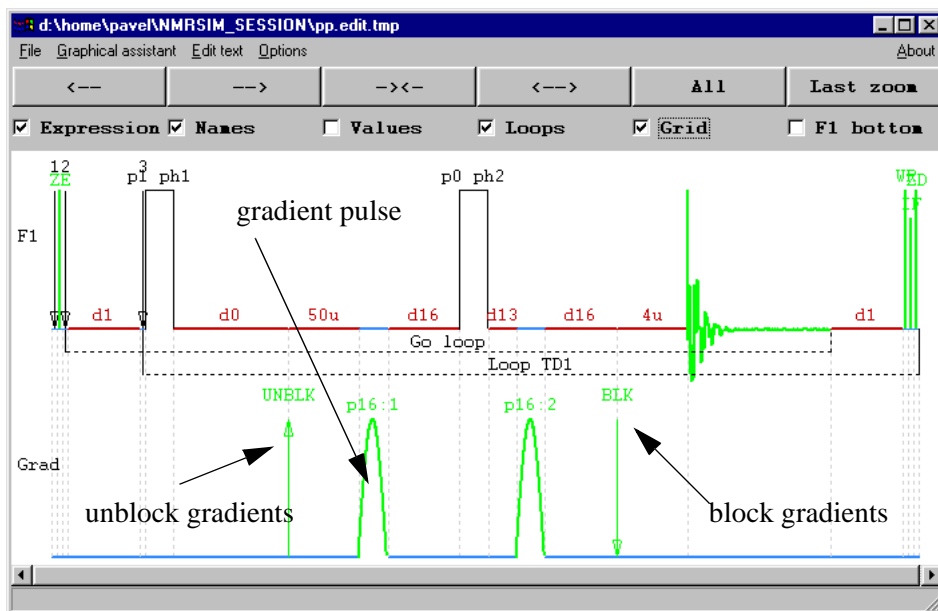
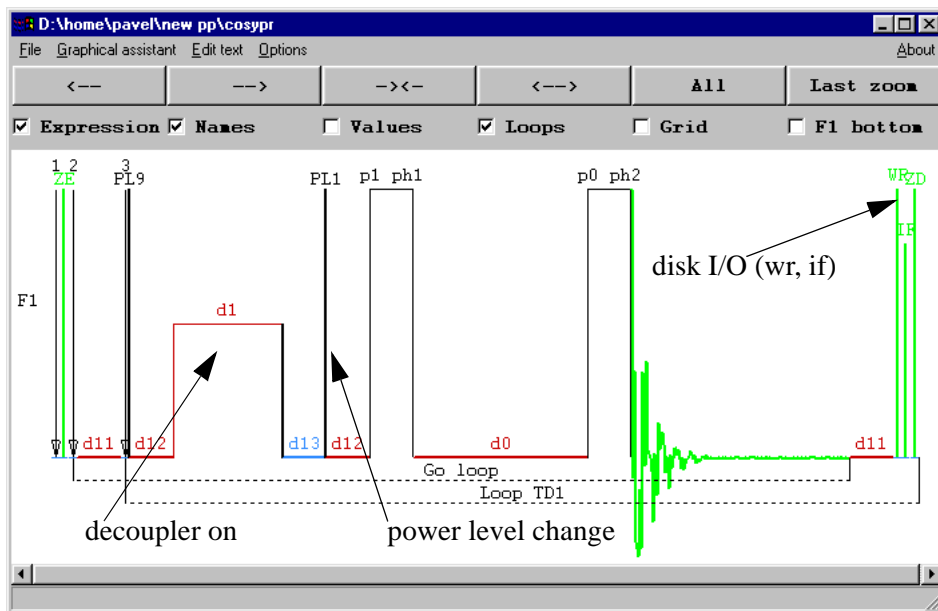
set using the ***-xconfig*** parameter (see “Parameter definitions” on page 18). The TOPSPIN command ***spdisp*** always reads the parameter values from the actual data

set.

5.5.3 Event symbols

Following pictures summarize the most important symbols used in the pulse program display.





5.5.4 Pulse trains, virtual channels

Pulse train is a part of pulse program, executing several pulses or delays simultaneously on one or more channels.

The pulse program *coloc* contains following line:

```
(d6):f1 (d0 p4 ph2):f2 (d0 p2 ph4):f1
```

There are two independent fragments which are executed on the same channel *F1*. NMR-SIM creates in such a case one additional “virtual” channel which allows to split visually the overlapping pulses and delays.

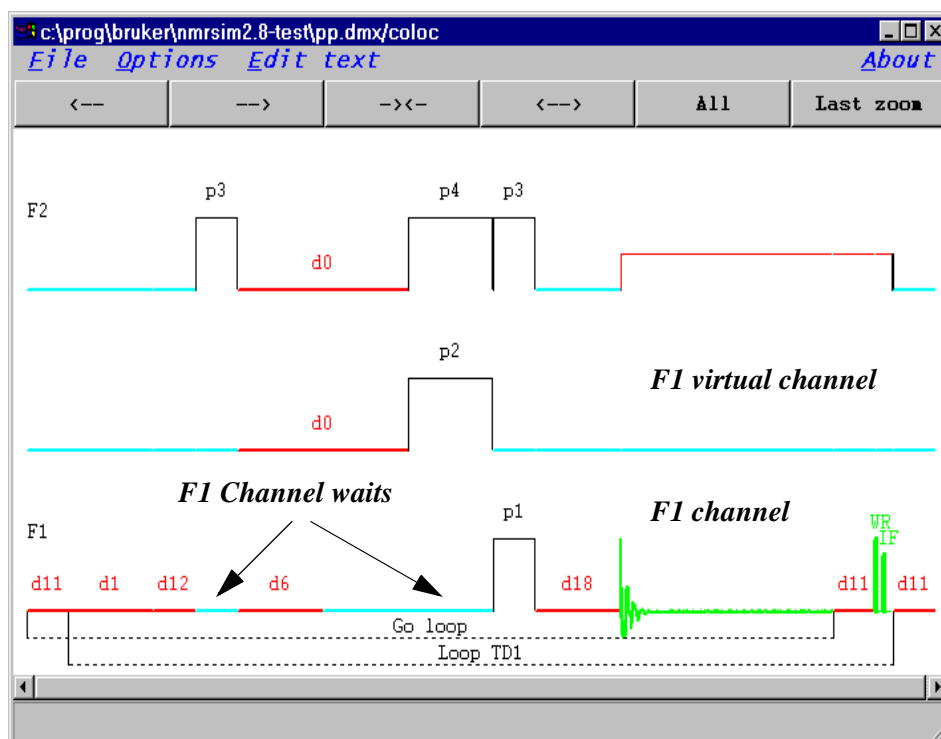
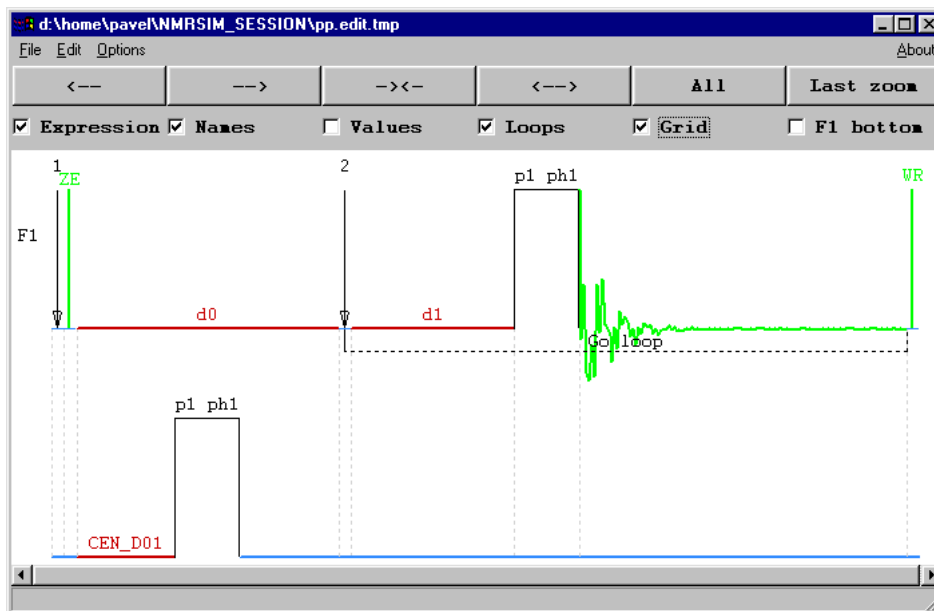


Figure 5.8 Virtual channel

5.5.5 Synchronization of events - grid

The grid lines shows, where the spectrometer synchronizes the actions between



channels. Each vertical dashed line is one synchronization event. This means, that all channels wait for the active channel. All action or events between the synchronization lines are executed in parallel.

5.5.6 Expressions in pulse programs

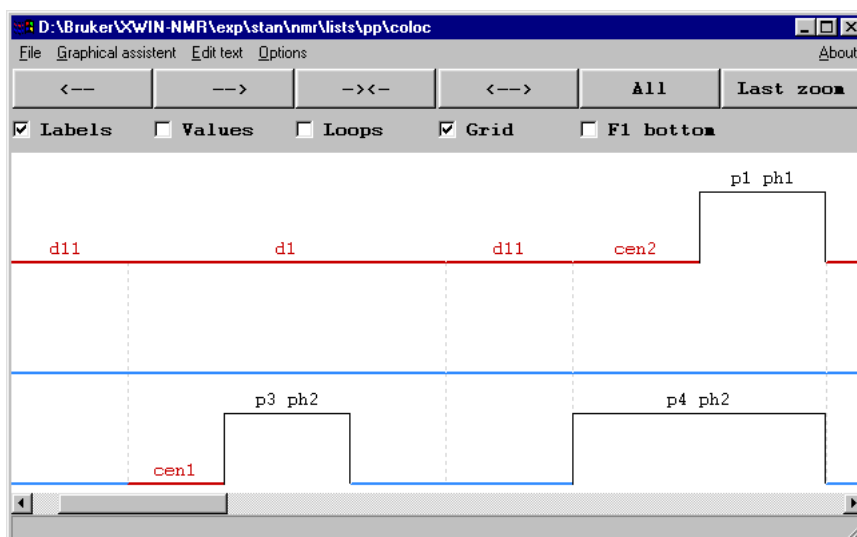
Modern pulse program may contain expressions which define the length of pulses or delays in the pulse program so, that the events fulfill some special alignment (centered, right aligned). NMR-SIM pulse program display may evaluate all expressions before first active command in the pulse program (first pulse, ze command,...). The evaluation of expression may be switched on or off using the **Expressions** toggle in the pulse program windows, or in the **Display** dialog. The symbolic width of the pulse program elements are used for the calculation, so the pulse program display shows the true event alignment.

Example: the following pulse program fragment uses a user defined delay *cen1* to center the pulse *p3* and the delay *d1*. The delay *cen2* is used to achieve the right

alignment between p1 and p4:

```
define delay cen1
define delay cen2
"cen1=(d2-p3)/2"
"cen2=(p4-p1)"

(d1):f1 (cen1 p3 ph2):f2
d11
(cen2 p1 ph1):f1 (p4 ph2):f2
```



5.6 Display of 3D gradients

The pulse programs using gradients for NMR imaging or tomography may be also shown in the pulse program display. In the Paravision environment is NMR-SIM also able to read the imaging parameters stored in the corresponding method files. To do it is necessary to specify an additional command line parameter **-tomo**:

```
nmrsim -tomo /u/example/nmr/ex/1/pdata/1  
-xconfig /d/example/nmr/ex/1/acqus -showp pulseprogram
```

This command initializes the paravision interface, reads the status parameters from

the data set and displays the pulse program. The display window contains additional buttons used to control the display of gradients:

- **xyz**
switch between the logical coordinates used for gradients (read, phase, slice) and the physical coordinates (x, y, z). The transformation used to get the physical coordinates is described in details in the Paravision manuals.
- ***2 /2 Reset**
Buttons used to vertically scale the display of 3D gradients.

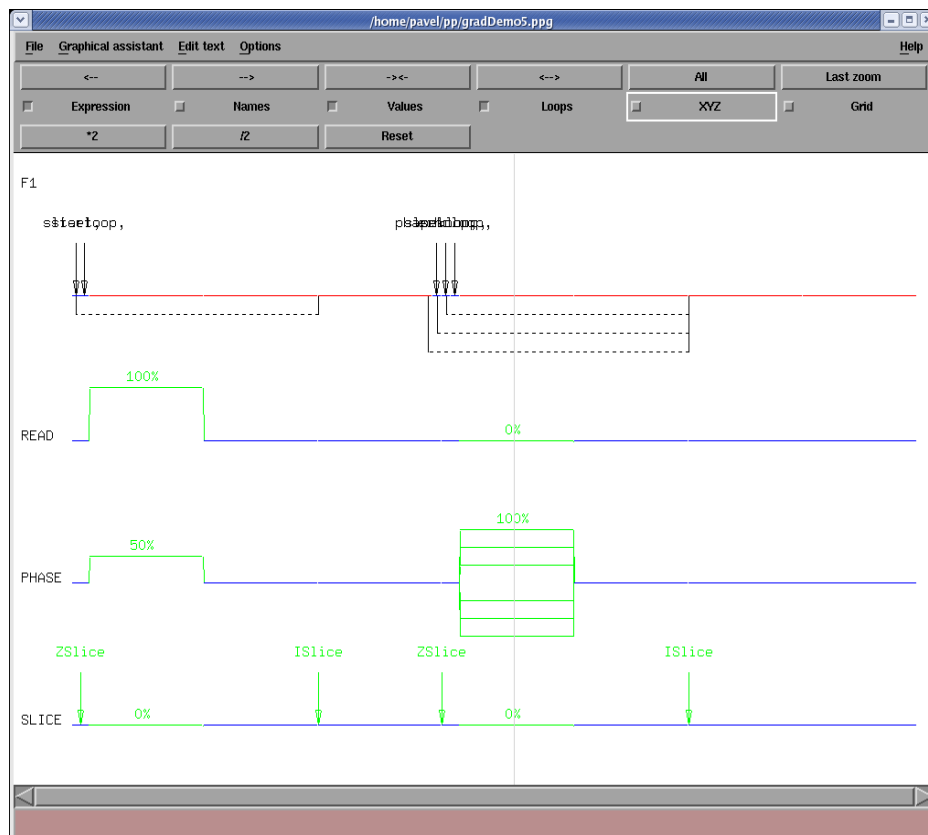


Figure 5.9 Example pulse program using 3D imaging gradients