TopSpin

Method Development
## Contents

- Pulse Programs
- Shapes
- Experiment Development & Simulation (NmrSim)
- AU Programs
- Python Programs
- Macros
- Pulse Programs In Python
- Plot Layout Programming
- User-Defined Command Panels

> Please click on a topic to view page
Pulse Programs

- Simulation of pulse generator output for pulse program development & testing
- Symbolic display of pulse program
Shapes

ShapeTool to define shaped pulses

2 ShapeTool exam2d_HH 1 1 C:\Bruker\TOPSPIN guest

Open
1274  NPOINTS
Inversion  EXMODE
180.0  TOTROT
32.034000  BWFAC
0.140491  INTEGFAC
0  MODE

Edit Shape Parameters

Phase

F1 [ppm]
F2 [ppm]

[points]
Shapes

Calculation and display of excitation profiles

- Define and manipulate a shape
- Display shape above spectrum
- Compute excitation profile and display above spectrum
Experiment Simulation (NmrSim)

Simulates a wide range of NMR experiments

Simulation result is a 1D, 2D, ... fid

Simulates the behaviour of general homo- and heteronuclear spin systems (up to quantum number 2)

Supports simulation of rotating frame magnetization transfer experiments (TOCSY or HOHAHA)

Supports simulation gradient enhanced exp.

Solves the quantum mechanical Liouville equation
The Bloch module lets you visualize the time development of the nuclear magnetization during various experiments.

The time evolution of a nuclear magnetization vector during an adiabatic pulse, calculated for several offsets, is shown as a projection on the sphere.
Experiment Simulation (NmrSim)

Time evolution of the magnetization shown in TOPSPIN
The proton spectrum of ethanol at 200 MHz. The inset shows the C13 satellites (vertical scale with 8 times magnification).
Experiment Simulation (NmrSim)

Comparison of simulated 13C DEPT spectra for three different leading pulses P0.

a) $P_0 = 45\, \text{d}$

b) $P_0 = 90\, \text{d}$

c) $P_0 = 135\, \text{d}$
Comparison of J-resolved spectra on 300 MHz and 600 MHz shows the significant reduction of *strong coupling artifacts* for the higher resonance frequency.
What is an AU (Automation) program?

A C program automatically interfaced to TopSpin

Purpose:
Extending TopSpin with user-defined functionalities, programmed in C

Example:
Requests LB,
performs em, ft, pk on the current dataset

double lb = 0.3;

GETCURDATA
GETDOUBLE ("Enter LB: ", lb)
STOREPAR("LB", lb)
EM
FT
PK
QUIT
AU Programs

AU development tools delivered with TopSpin

GNU C Compiler
For Windows or Linux

AU Browser
AU Library

AU Editor
TopSpin supports: *Python programs automatically interfaced to TopSpin*

**Purpose:**

*Extending TopSpin with user-defined functionalities, programmed in Python ("Jython")*

**Example:**

*Requests LB, performs em, ft, pk on the current dataset*

```python
lb = INPUT_DIALOG("", "", 
    ["Please enter LB: "], ["0.3"])  
if lb == None: 
    EXIT() 
PUTPAR("LB", lb[0]) 
EM() 
FT() 
PK()
```
Python Programs

Python development tools delivered with TopSpin

Python Program Browser and Library

Jython Interpreter (Java variant of Python)
What is a Macro?
A sequence of TopSpin commands

Purpose:
Extending TopSpin with user-defined functionalities, built from existing commands

Example:
Sets LB, performs em, ft, pk on the current dataset
What is a Python Pulse Program?

A Python program acting as a Pulse Program

Purpose:
Computing pulse program parameters such as delays, shapes, phases using Python statements for the contained pulse program

Example:

Computes phase list `ph1` using Python and starts acquisition

```python
PPTEXT = ""
1 ze
2 dl
   pl phl
   go=2 ph31
exit
ph31=0 2 2 0 1 3 3 1 """

pulsprog=DEF_PULSprog(PPTEXT)
phl = [0, 0, 4, 4]*2 + [2, 2, 6, 6]*2
phlinx = 360/4
for i in range(16):
    phl[i] = float(phl[i])*phlinx
pulsprog.DEF_PHASE_LIST(1, phl, phlinx)
PUTPAR("PULPROG", "bgzg")
pulsprog.SAVE_AS("bgzg")
ZG()
```
What is a command panel?

A panel containing user-defined buttons to execute commands, AU programs, macros, etc.

Purpose:

Defining application specific user interfaces

Examples:

```
BLUE1=51$ 204$ 255
YELLOW1=255$ 255$ 0
GREEN1=84$ 196$ 20
# Title definition
TITLE=1D Processing Panel
TITLE_COLOR=0$ 0$ 255
# Toggle button definition
TOGGLE_BUTTON=To 2D
TOGGLE_CMD=bpˉn bproc2d
TOGGLE_TIP=Switch to 2D processing
# Top row button definition
TOP_BUTTONS=EM$ $FT$ $PK$ 
TOP_COLORS=yellow$ yellow$ yellow$ yellow
TOP_CMDS=em$ ft$ pk
TOP_TIPS=Exponential multiplication \ Fourier transform\nPhase correction
```