

University of Colorado 800 MHz NMR Facility

Creating Shaped Pulses with Pbox

This document contains step by step instructions for creating shaped pulses using Pbox along with some tips to simplify the procedure and get good results. This document covers using Pbox at the Unix command line and then using the new graphical interface in VNMRJ.

Before You Start

Before you can create a shaped pulse, you'll need to have calibrated a good reference 90° pulse for the nucleus in question, preferably at a power level reasonably close to the power your shape will require. If you know the approximate pulse width your shaped pulse will have, you can estimate the power using the 'attval' or 'cpower' macros. If you have no idea, you can create the shape using your hard pulse calibration, note the power level it tells you to use, and then re-create the shape after doing a calibration at that new power level.

What Shapes Can You Create?

There are a fairly large number of possible pulse shapes that Varian groups into a number of categories. The most commonly are excitation (90° pulses), inversion and refocusing (180° pulses), and decoupling, although there are others. The names of the various shapes and the parameters Pbox needs to create the waveforms are stored in /vnmr/wavelib. Please note that at 800 MHz and higher you will have to use adiabatic pulses and decoupling if you want to span large bandwidths without damaging the instrument or probe, especially for ¹³C experiments.

Running Pbox from the Command Line

My preferred method of running Pbox was from the Unix command line. This method is very general and provides good results in most cases. The basic syntax for a pulse or decoupling pattern with a single waveform is as follows:

```
Pbox filename -w 'waveform bw(/pw) offset' -p ref. power -l ref. pw90
```

where

- filename*: the name of the pulse you are creating, Pbox will append .RF or .DEC depending on the waveform. The file is placed in your shapelib.
- waveform*: the name of the waveform from /vnmr/wavelib
- bw(/pw)*: the bandwidth (in Hz) and/or the pulse width (in seconds) that you want your shaped pulse to have. Pbox may change these slightly.
- offset*: how far to shift the pulse. Omit or set to zero for on-resonance. Positive offsets are in the downfield direction
- ref. power* and *ref. pw90*: from the reference 90° pulse you've calibrated

The above syntax is the most basic and most commonly used. Pbox has many other options that are described in the "VNMRJ Liquids NMR User Guide".

Example - create a reburp pulse on ¹³C with a bandwidth of 1 kHz and shifted 2 kHz downfield. Assume you calibrated a soft 90 degree pulse width of 55 μs at 48 dB. Type:

```
Pbox my_reburp_pulse.RF -w 'reburp 1000 2000' -p 48 -l 55
```

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Creating a Pulse with Multiple Excitation or Decoupling Bands

It is possible to create a shape in Pbox that combines more than one waveform to pulse or decouple different portions of your spectrum, but you can not put more than one wave string in a single command. You can, however, put as many waveforms as you like into a file named Pbox.inp that lives in your vnmrsys/shapelib directory. Pbox will generate a shaped pulse with the parameters in this file called with no arguments (*i.e.* you simply type 'Pbox' at the Unix command line). Below are the contents of a sample Pbox.inp file that will create a dual lobed G3 inversion pulse named dual.RF in your shapelib with one lobe covering 5 kHz on resonance and the other covering a 2 kHz bandwidth shifted 15 kHz downfield (important lines shown in red).

```
Pbox.inp file.
  For more information see man('Pbox')
*****
  Pbox parameters : name, steps, dres, maxincr, attn,
                    stepsize, sfrq, refofs, sucyc, reps, header, bsim,
                    T1, T2, sw, dcyc, type, bscor, ref_pwr, ref_pw90.

      name          = dual
~~~~~Waves~~~~~
  sh  bw(/pw)  ofs  st  ph  fla  trev  d1  d2  d0
~~~~~
{ g3 5000 }
{ g3 2000 15000 }

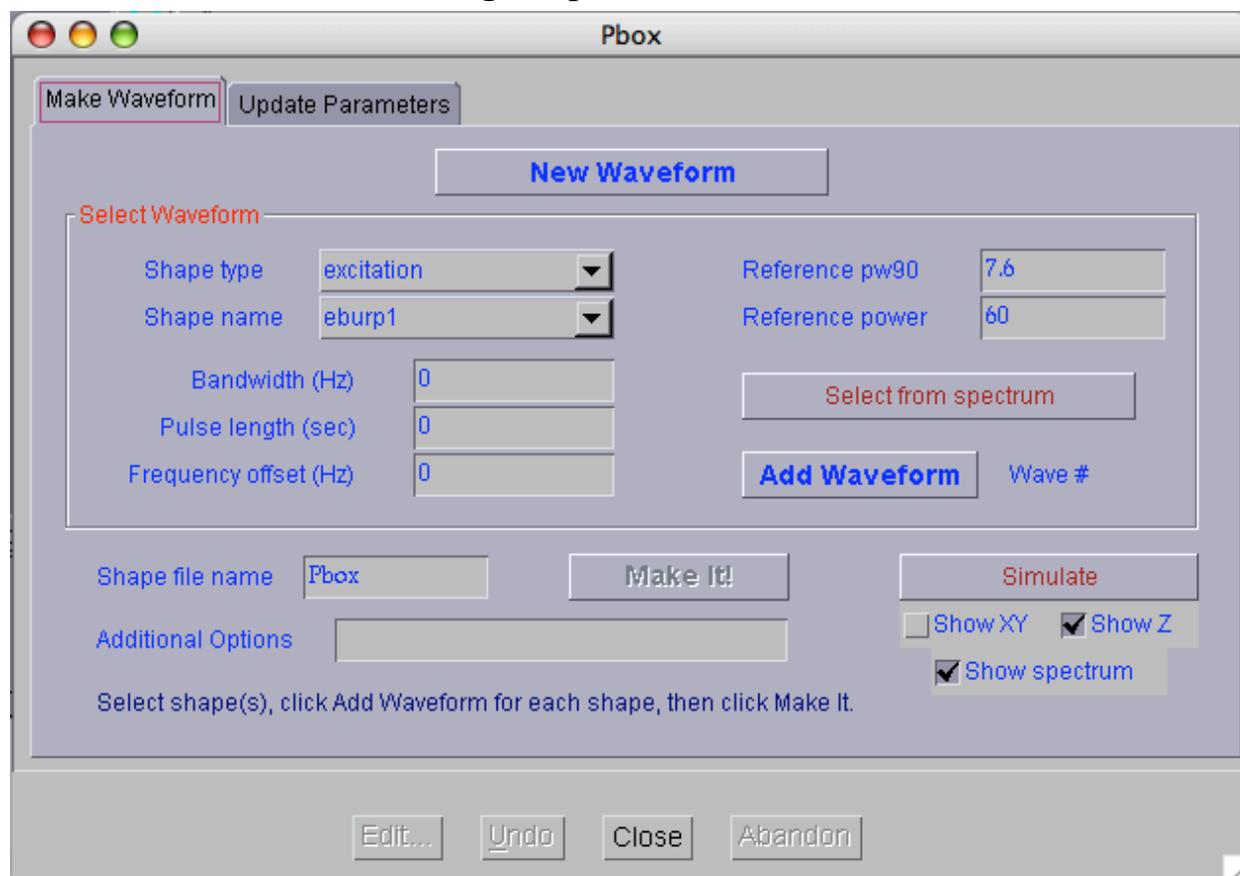
RF Calibration :
-----
      ref_pwr      = 60
      ref_pw90     = 14
```

Please be aware that when combining many waveforms, especially those that cover relatively large bandwidths, the power level required by the resulting pulse may be large. Be careful not to put long, high power pulses into the probe.

Simplifying Your Life: Using VNMRJ's Graphical Interface to Pbox

One of the nicer improvements introduced with VNMRJ is a graphical interface to Pbox that allows you to enter all the information discussed above in a convenient and straightforward manner. To call up the Pbox interface, select 'Pbox' from the 'Process' menu in the native VNMRJ interface. This will bring up a mostly blank window; click on the 'New Waveform' button to continue, which will bring up the rest of the interface (see image on next page). Select the shape type and name from the pull down menus, fill in the pulse and reference information including the name you want your new pulse to have, and then click the "Add Waveform" button. As soon as you add a waveform, the "Make It!" button will become active. You can push this button to make the shaped pulse now, or you can add more waveforms first. The new shape will be stored in your shapelib. You can look at the new shape's profile in VNMRJ's spectrum display window by clicking the "Simulate" button if you wish to.

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If You Forget the Parameters for Your Shape

One really nice feature of Pbox is that it puts a descriptive header at the top of each shaped pulse file that it creates. The header contains all the information you used to create the pulse as well as the correct pulse width and power level to use in your pulse sequence. If it's been a while since you created the pulse, you may find it useful to go back and make sure the shape was created using a reasonable reference parameters.