# Classical simulations with PJNMR
# BCMB/CHEM LAB
# 01/25/12

The program PJNMR was written by Paul-Jean Letourneau as a joint project between the PENCE & NANUC projects in Canada. It rotates vectors representing spin magnetization by RF pulses and evolution times. It also has a graphical depiction of the density matrix elements associated with each state (you will learn more about density matrix representations later). It allows up to 3 spins and provides a history and schematic of the pulses applied, thus creating a 'pulse program', which can be saved as a macro. It is a java applet and so can be run on any platform. If you want a copy for your own computer, follow the download instructions under "download" on the www.nanuc.ca website. You will have to register, but this is free. Follow the installation instructions. There is an install script which will set up appropriate links, etc.

**Start up**.

Getting started will vary somewhat depending on how the software was installed. i) If you downloaded it yourself to a particular directory on a windows machine, you should find a "pjnmr.app" subdirectory there. Follow down through "contents", "resources", and "java". You should find a "PJNMR.jar" file. If you click on this, pjnmr will start.
ii) If you are using a program setup for course use under a LINUX system, open a terminal window as you did in the LINUX introduction. You can look for the program using the "ls" command. It is likely to be in a directory set up on the server that can be accessed by all (/programs). In this case, you could start pjnmr by typing the full path to the program (for example: /programs/pjnmr/pjnmr). However, at UGA a "source" command has been put in your .cshrc file that directs your system to look in and execute commands from a directory where the alias "pjnmr" has been defined. So, just type "pjnmr".
iii) When you successfully start the program you should get the following screen ( fig.1)

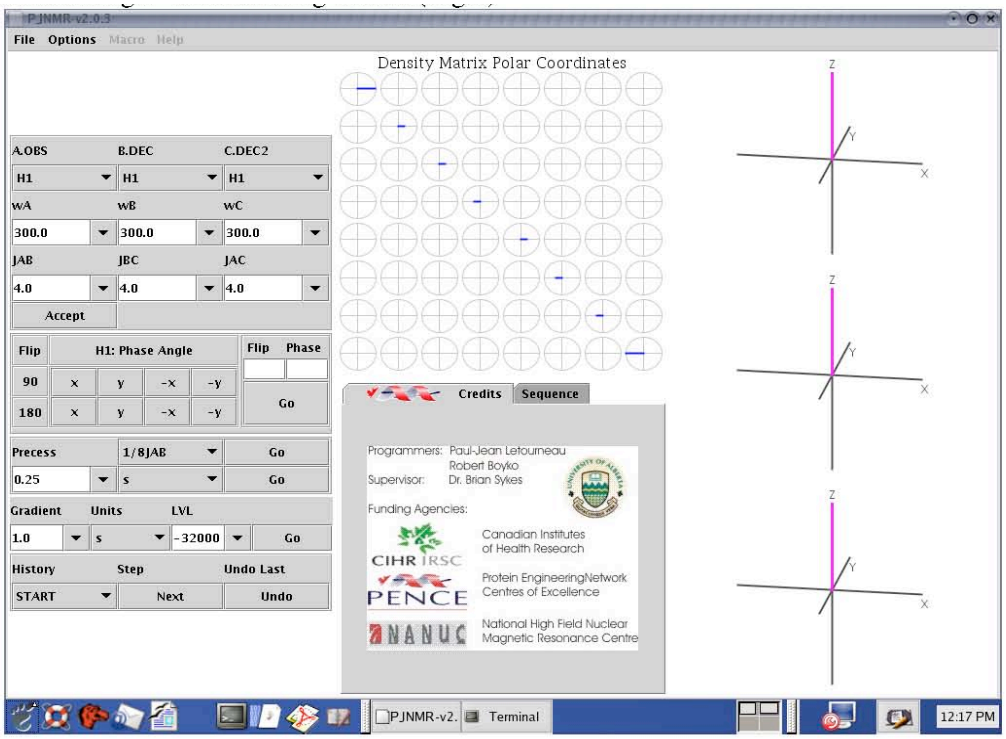



fig. 1

**General Operations.**

Set up standard spin systems with pulldown menus. Custom values can be entered in the boxes. NOTE: for 'rotating frame' behavior, one of the precession values ( e.g. wA) should be set to zero. The Accept button will initialize the chosen spin system. Accept button will always return to the initial conditions set above.

Flip: angles can be chosen with buttons, or entered in the boxes. E.g. Flip=90 and Phase=0 is equivalent to 90 x.

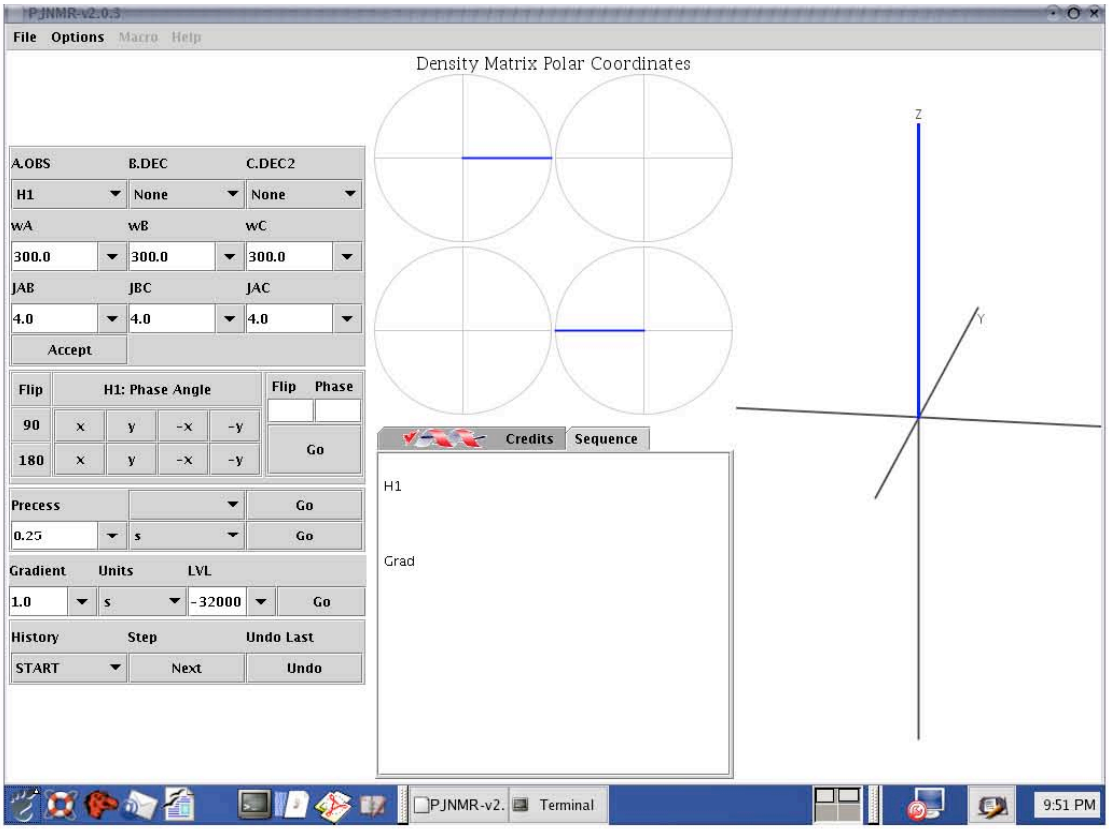
Precess: For a single spin, only evolution times are possible, and can be entered in the box. If a multispin system is created, the upper menu allows convenient times like 1/4JAB.

Command History: keeps track of your actions. You can return to START or any point in the history by pulling down the menu and clicking on a line. Clicking on Next will step
through the history. Undo Last and Undo allow for editing. One can save the history of commands at any time during the session or when exiting the
program. The macro of saved commands can be rerun at a later session.

**Exercise 1.**

Effect of a 90 x pulse on equilibrium +Z magnetization.
Setup a single spin system:
1) pulldown the H1 menu under B.DEC and choose none; repeat for C.DEC2. Click on 'Accept'. Click on the 'Sequence' tab of the box in lower center of your screen to bring it forward.
-the display should be as shown below in fig. 2.
-for the interested student, notice the density matrix only has elements in the diagonal. i.e. Full populations , no coherence yet.
2) Click on 90 x. You will see the vector move from +z to -y. You will also see a schematic pulse drawn in the sequence box.
(To get a pseudo movie effect, initialize with Accept, then choose Flip=5 and phase=0. Repeated clicking of Go will show the movement of the vector.)
Note the density matrix shows only off-diagonal elements of the -1 quantum coherence with a phase related to the X-axis.
Note that the convention used is that positive pulses give clockwise rotations – this means that the B1 field of a 90x pulse is applied along the –x direction.

Fig 2. Display of initial +Z state of single spin (A.OBS)



**Exercise 2.**

Repeat the above with 180x and other angles ( 90y, 270y, etc.).

**Exercise 3.**

Effect of pulses on x and y magnetization.
Bring the vector to the +X position by clicking on Accept, then 90 y. Consider this as your new starting position. Try another 90 x. Repeat with 'starting' positions of -X, +Y, -Y.

**Exercise 4.**

Composite pulses . e.g. compensated 180s
i) Reinitialize with accept. Using the Flip and Phase boxes to enter values, compare an accurate 180: Flip=180 Phase=90 (i.e. 180 y) with a poorly calibrated 180 ( or different '180' due to offset effects) Flip=170 Phase=90 ( i.e. 170 y)
ii) Reinitialize with accept. Compare the same calibrated and uncalibrated pulses, except by using a composite 180 y pulse = ( 90y 180-x 90y )
(a) Flip=90 Phase=90 Go; Flip=180 Phase=180 Go; Flip=90 Phase=90 Go. (equals 180 y)
(b) Flip=85 Phase=90 Go; Flip=170 Phase=180 Go; Flip=85 Phase=90 Go. ( equals 170 y)

**Exercise 5.**

Precession.
i) Change wA = 100.0, then Accept, then Flip 90 x.
ii) The default Precess value is 0.25 s. Click on the Go on the same line.
What happens?
iii)repeat (i) then change Precess value to 0.125 s, Go.
iv) Repeat (i) then change Precess value to 0.001 s, Go and repeat Go.
Change the larmor (wA) frequency and try different precession delays.

**Problem set L1.**

1. Effect of pulse angle. Starting with Iz magnetization, what is the final state of I after:
a) a 90 x pulse b) a 270 x pulse and c) a 720 x pulse?
2. Effect of pulse phase. Starting with Iz magnetization, what is the final state of I after:
a) a 90 y pulse, b) a 270y pulse, c) a 90 -y pulse, and d) a 270 -x pulse.
3. Effect of initial magnetization. Give the final state of I for the following cases:
90y
Ix-->
90x
Ix-->
270y
Iy-->
180z
Iy-->
4. Composite pulses. 'Volume selective' 90 degree composite pulse: (90y 90-x 90-y 90x). This pulse was designed for removing remnants of strong solvent signals that arise from sample outside of the nmr coil volume. These signals are poorly shimmed and have very low pulse angles ( e.g < 20 degrees) . For strong solvent signals, they can interfere with weaker signals of interest (e.g. broad asymmetric base of solvent peak) . Try comparing a 'good' 90 ( found inside the coil volume) with a 'poor' 90 ( e.g. a 20 degree pulse) found outside the coil volume. -i.e. Flip=20 Phase=90 Go; Flip=20 Phase=180 Go, etc.
How does this composite pulse solve the problem?