Classical simulations with PJNMR.
This program 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. 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.
Unlike PENCIL, there is no simulation mode and no way to demonstrate chemical shift offset effects.

Download it.
It is a java applet and so can be run on any platform.
Download the tar file from www.nanuc.ca (e.g. see PJNMR icon on the right) and follow the installation instructions. There is an install script which will set up appropriate links, etc.

Start up.
After setting up a pjnmr_v2.03 directory, you can either
i) cd to the directory and type 'java -jar PJNMR.jar' as described
ii) or if the install scripts were used, simply type a single command such as 'pjnmr'.
You should get the following screen (fig.1)

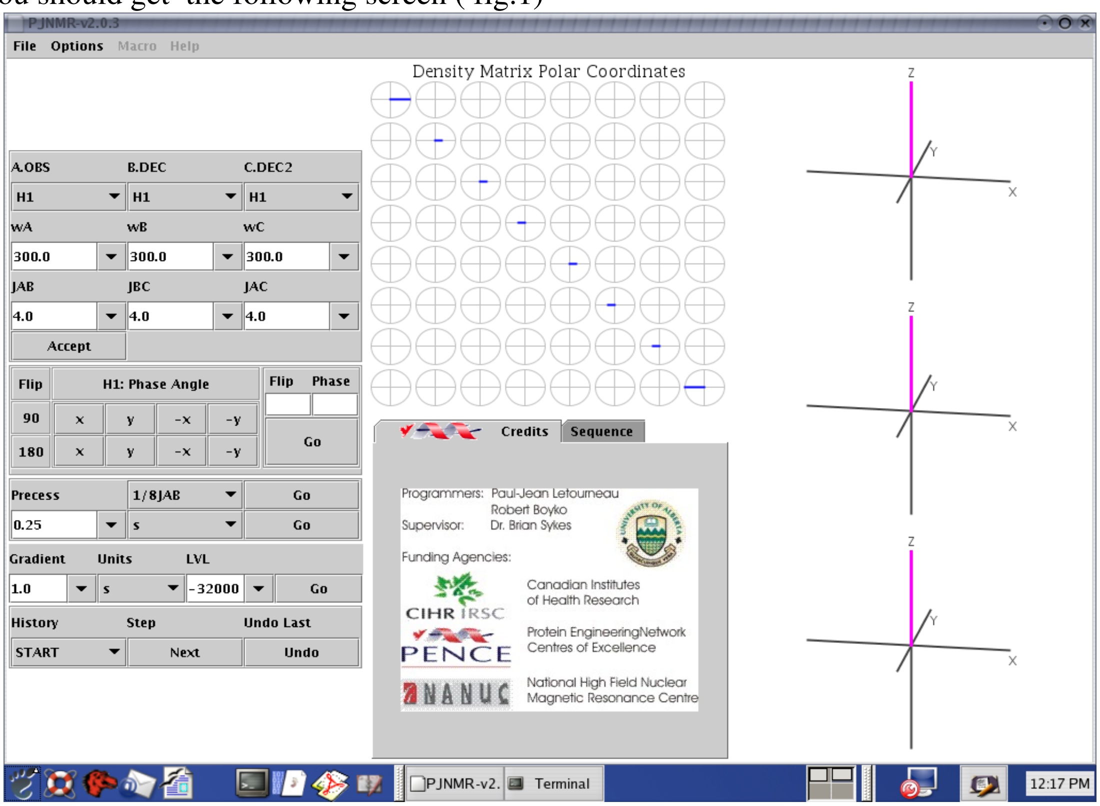


fig. 1

General Operations.

Set up standard spin systems with pulldown menus. Custom values can be entered in the boxes. NOTE: for 'rotating frame' behaviour, 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.

History: keeps track of your actions. You can return the the 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 90 x pulse on equilibrium +Z magnetization.

Setup single spin system:

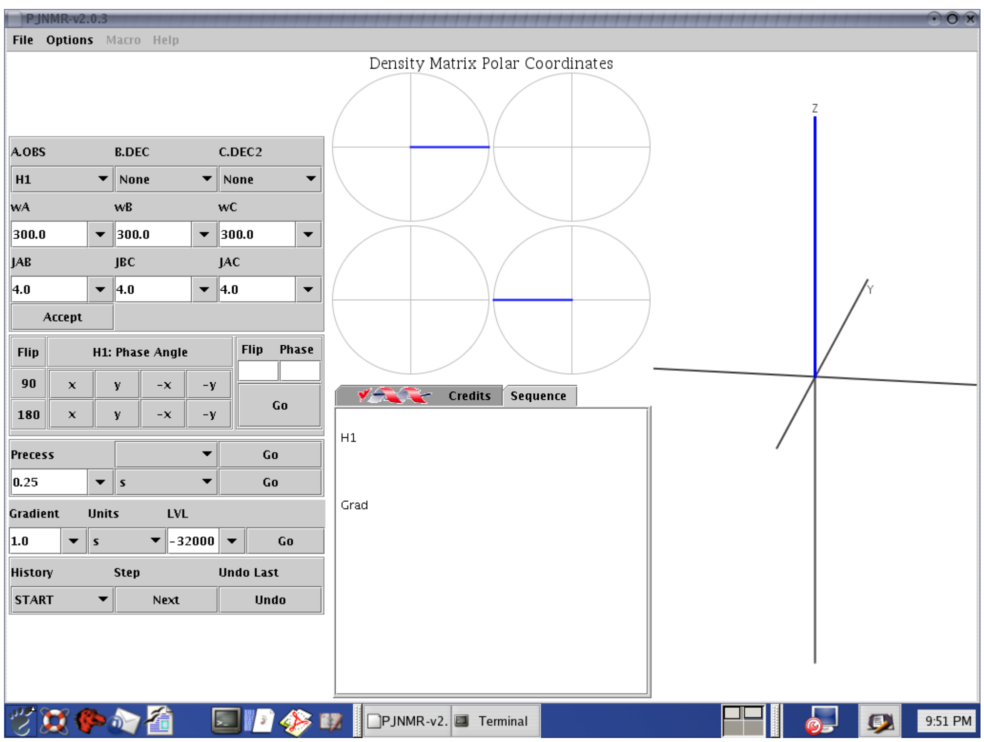
1) pulldown the H1 menu under B.DEC and choose none; repeat for C.DEC2.
   Click on 'Accept'. Click on the 'Sequence' page (box to the right) to bring it forward.
   -the display should be as shown below in fig. 2.
   -for the interested student, notice the density matrix only has elements in the diagonal.
   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.

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



Exercise 2. Repeat above with 180x and other angles (90y, 270y, etc.).

Exercise 3. Affect 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 4. Precession.
i) Change wA = 500.0, 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 0.025 s, Go and repeat Go.

Change the larmor (wA) frequency and try different precession delays.

Problem set #2.

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?