Assignment 6 is due Friday, Nov 21.

Background:
a. Look in the Mathematica Index of Functions for FourierTransform.
b. Look also for the function Piecewise
c. Create a function (not necessary to hand this in) that satisfies the following:
f(t) = t^2 $(t < 0)$
= t $(t > 0)$
d. Read the signal processing chapter posted.
e. Read the nmr readings posted.

1. (from Keeler)
a. In a 1H NMR experiment, the peak from TMS is found to occur at 500.134271 MHz. Two other peaks in the spectrum are found at 500.1350021 and 500.137921 MHz; compute the chemical shifts of these two peaks in ppm.

b. Given the receiver reference frequency ν_{rx} is 500.135271 MHz, recompute the chemical shifts of the two peaks using the equation:

$$\delta_{ppm} = 10^6 \times \frac{\nu - \nu_{TMS}}{\nu_{rx}}$$

Does this make a significant difference to the value of the shifts?

c. What would the frequency separation, in Hz and in rad/s, be between these two peaks if the spectrum were recorded using a different spectrometer which operates at 400 MHz for protons. The receiver reference frequency for this spectrometer is $\nu_{rx} = 400.130000$ MHz.

2. Calculate (numerically, using Mathematica) the fourier transform of the following cases.
Choose f=20 Hz. Plot the function if it is possible to do so.

a. A sinusoidal function S(t) = a*sin(2*Pi*f*t) (t>0)

b. A sinusoidal function truncated at t=0.5s (a piecewise function that is sinusoidal below t=0.5 and zero above)

c. Define a square ("hat") pulse that satisfies
h(t) = 1 for $-\tau < t < \tau$
= 0 otherwise
where $\tau = 10\,\mu s$
(Possibly useful hint: in the piecewise function you can make requirement on t^2 instead of t)
Calculate and plot the Fourier transform for this hat function. Be careful to plot the full y extent of the function. Show the shape of the FT over frequency ranges of 0 -10 MHz, 0 -1 MHz, 0-100 kHz and 0-10 kHz.

3. Fourier transform of a square rf pulse.
Check in 2c. to confirm that over a 10 ppm range on the 500 MHz spectrometer, that the fourier transform of the $\tau = 10\,\mu s$ "hat" RF pulse is fairly flat. Comment (1-2 sentences) on why this is

desirable.

4. Your NMR data

Your NMR data is uploaded in ascii file format (and a name with your initials) to the course webpage.

a. Plot your time-domain signal (the "fid").

b. Calculate and plot its Fourier transform (the "spectrum").

c. Multiply the fid by a trial phase factor (exp(i*Phi)) and plot the spectrum for the value of phi that gives pure absorption lineshapes and for the value of phi that gives pure dispersion lineshapes.

5. Power Spectrum and Signal-Noise

In signal processing one often deals with the "power spectrum" of the signal or the noise. Find out what it is.

a. Plot the power spectrum from the Fourier transform of the fid in Question 4.

b. Based on the fact that the fid decays in a short time, but the noise extends for all times, find a systematic way to calculate the signal-to-noise ratio for your data. Outline your approach. Calculate the signal to noise ratio for your data (state your answer in decibels).