

FREE INDUCTION DECAY: An MLAB Example

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Introduction

Consider the following experiment: a 1 cubic centimeter sample of water at room temperature is placed between the pole faces of a 10,000 Gauss (1 Tesla) electromagnet. As the system reaches equilibrium, a small magnetic dipole of magnitude $3.4\text{E-}6$ Gauss is induced in the sample parallel to the applied field. Designate the axis passing from the south pole to the north pole of the magnet as the z-axis with the origin at the center of the sample, midway between the magnet's pole faces. The sample is surrounded by two thin wire coils such that the axes of the coils are perpendicular to each other and to the z-axis. The axes passing through the center of the coils are designated the x and y axes. A brief 42 megahertz alternating current pulse is applied to the x-axis coil. If the pulse is of the appropriate amplitude and duration, it causes the induced magnetic dipole to tilt away from the z-axis. The magnetic dipole then precesses around the z-axis, gradually returning to its equilibrium position parallel to the z-axis. The component of the magnetic dipole which rotates in the xy-plane induces 42 megahertz oscillating voltages—90 degrees out of phase—across the terminals of the two coils which die away in time.

These signals are termed *free induction decay signals* and they are the basic physical effect which underlies modern day magnetic resonance imaging (MRI) and nuclear magnetic resonance (NMR) experiments. Free induction decay can be described by a model developed by F. Bloch in the paper “Nuclear Induction” Phys. Rev. 70 (1946) 460. The mathematical formulation

of the model is called *Bloch's equations* and consists of 3 ordinary differential equations:

$$\frac{dM_x}{dt} = \gamma(M_y H_z - M_z H_y) - \frac{M_x}{T_2} \quad (1)$$

$$\frac{dM_y}{dt} = \gamma(M_z H_x - M_x H_z) - \frac{M_y}{T_2} \quad (2)$$

$$\frac{dM_z}{dt} = \gamma(M_x H_y - M_y H_x) + \frac{(M_0 - M_z)}{T_1} \quad (3)$$

These equations predict the evolution of the induced magnetic dipole, $\mathbf{M}(t) = (M_x(t), M_y(t), M_z(t))$, in the presence of a uniform magnetic field $\mathbf{H} = (H_x, H_y, H_z)$, where M_0 is the equilibrium magnitude of the induced magnetic dipole, γ is the gyromagnetic ratio for protons, T_1 is the spin-lattice relaxation constant, and T_2 is the spin-spin relaxation constant. The free induction decay signals observed on the x-axis coil and y-axis coil are proportional to the components $M_x(t)$ and $M_y(t)$, respectively.

This paper will demonstrate how the MLAB mathematical modeling system can be used to solve Bloch's equations to predict free induction decay signals in single and double pulse experiments. MLAB is a computer program whose name is an acronym for "Modeling LABORatory". It is an interactive interpreter like Basic but with sophisticated instructions for solving ordinary differential equations, curve fitting, and generating publication quality graphs. It was originally developed at the National Institutes of Health. It is available from Civilized Software for a variety of computer platforms including DOS-based IBM compatible personal computers, Macintosh II's, and SUN, NeXT, and SGI Unix workstations.

A Single $\frac{\pi}{4}$ Pulse Experiment

To begin using MLAB, double click on the MLAB icon—if running an operating system with a graphical user interface, or type `mlab` at the operating system prompt for DOS or Unix systems. MLAB then types some initialization information on the screen and an asterisk, `*`. The asterisk is the prompt for the user to type MLAB instructions. In what follows, MLAB instructions will be typed in **bold face** on lines beginning with `*` and comments will be delimited by `/*` and `*/`. Although it is not shown, the `<Enter>` key should be struck at the end of each line.

We begin by simulating a single pulse experiment which rotates the magnetic dipole of the sample by $\frac{\pi}{4}$ radians about the x-axis. First define Bloch's equations by typing:

```

* function mx't(t) = g*(my*hz(t)-mz*hy(t))-mx/t2
* function my't(t) = g*(mz*hx(t)-mx*hz(t))-my/t2
* function mz't(t) = g*(mx*hy(t)-my*hx(t))+(m0-mz)/t1

```

The `function` statement allows the user to define any algebraic or differential equation model desired. The apostrophe, `'`, denotes the differentiation operation.

Next assign values to the constants appearing in the `function` statements by typing

```

* g = 2.66E4      /* gyromagnetic ratio for protons */
* m0 = 3.4E-6     /* equilibrium magnitude of magnetic dipole in Gauss */
* t1 = 1.E-6      /* spin-lattice relaxation time in seconds */
* t2 = 1.E-6      /* spin-spin relaxation time in seconds */
* beta1 = pi/4    /* rotation angle for first pulse in radians */
* h0 = 10000      /* magnitude of external magnetic field in Gauss */
* fct hx(t) = 0   /* x-component of external magnetic field in Gauss */
* fct hy(t) = 0   /* y-component of external magnetic field in Gauss */
* fct hz(t) = h0/* z-component of external magnetic field in Gauss */

```

The magnetic field is defined as having only a z-component of 10000 Gauss. For a normal water sample, T_1 is roughly 1 second and T_2 is roughly a millisecond. Fictitious values for the spin-lattice and spin-spin relaxation constants have been selected here so that the effect of relaxation can be observed in the time scale of several precessions of the induced magnetic dipole.

The magnetic dipole vector will precess about the z-axis at the Larmor frequency, $\omega = \frac{\gamma H_0}{2\pi} = 42$ megahertz. We will solve Bloch's equations for ten precessions sampled at 300 time points. Define a vector `t` with components equal to the times of observation.

```

* nsteps = 300
* tau = 10*2*pi/(g*h0)
* t = 0:tau!nsteps

```

The `-:-!` construct in the last statement instructs MLAB to make `t` a row vector with components 0 to `tau` in 300 steps. We can now simulate the single pulse experiment by defining a so-called *macro* which initializes the components of the magnetic dipole vector at time 0 after the pulse and then integrates the differential equation model.

```
* pulse1 = "initial mx(0) = 0;\
            initial my(0) = sin(beta1)*m0;\
            initial mz(0) = cos(beta1)*m0;\
            m = points(mx,my,mz,t);"
```

Here the `initial` statements provide the initial conditions for the differential equations—the equilibrium dipole moment is rotated by an angle `beta1` about the x-axis. The `points` operator solves the differential equations for `mx`, `my`, and `mz` at the times listed in `t`. The `points` operator returns a 4 column array with time in column 1, and the x, y, and z components of the magnetic dipole vector in columns 2, 3, and 4, respectively. The macro is executed as follows:

```
* do pulse1
```

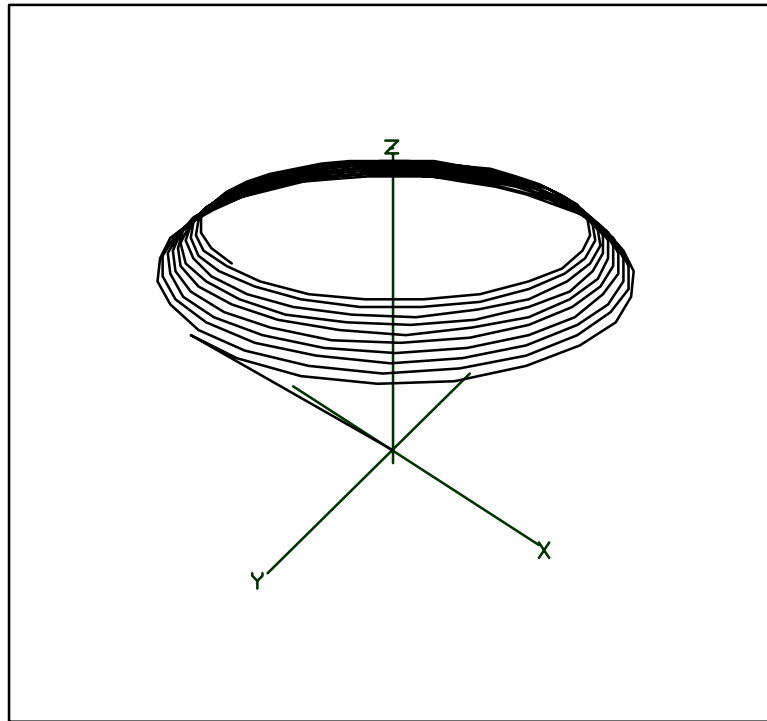
We can generate a 3 dimensional perspective figure of the time evolution of the magnetic dipole vector by defining another macro:

```
* mdip = "delete m col 1;\
          m = (0^^'3)&m;\
          draw m lt sequence;"
```

This macro instructs MLAB to throw away the time information in column 1 of the matrix `m`, add the origin (0, 0, 0) to the list of magnetic dipole vector components, and draw the resulting sequence of points. We execute the macro with some 3 dimensional perspective positioning commands as follows:

```
* do mdip
* cmd3d("raise 1")      /* raises the point of view */
* cmd3d("truck 1")     /* moves the point of view to the right */
* cmd3d("track")       /* points the direction of view to the center */
* cmd3d("dolly 1")     /* moves the point of view toward the subject */
* cmd3d("twist -20")
* cmd3d("axes")        /* draws coordinate axes */
* view
```

The following picture then appears on the display:



Note that the magnetic dipole at time 0 is drawn as a line segment at a 45 degree angle in the yz plane and that as time progresses, the head of the magnetic dipole vector precesses around the z-axis. As the vector precesses, the magnitude of the component in the xy plane (the transverse component) decreases in time at a rate determined by T_2 , while the component along the z axis (the longitudinal component) increases in time at a rate determined by T_1 . If the MLAB calculation of the magnetic dipole's time evolution were continued to longer times, the transverse component of the magnetic dipole would completely vanish and the magnetic dipole would fully recover along the z-axis.

The transverse component of the magnetic dipole can be decomposed into x and y components. It is the variations of the components of the magnetic dipole along the x and y axes which give rise to the free induction decay signals. These can be drawn by defining and executing another macro.

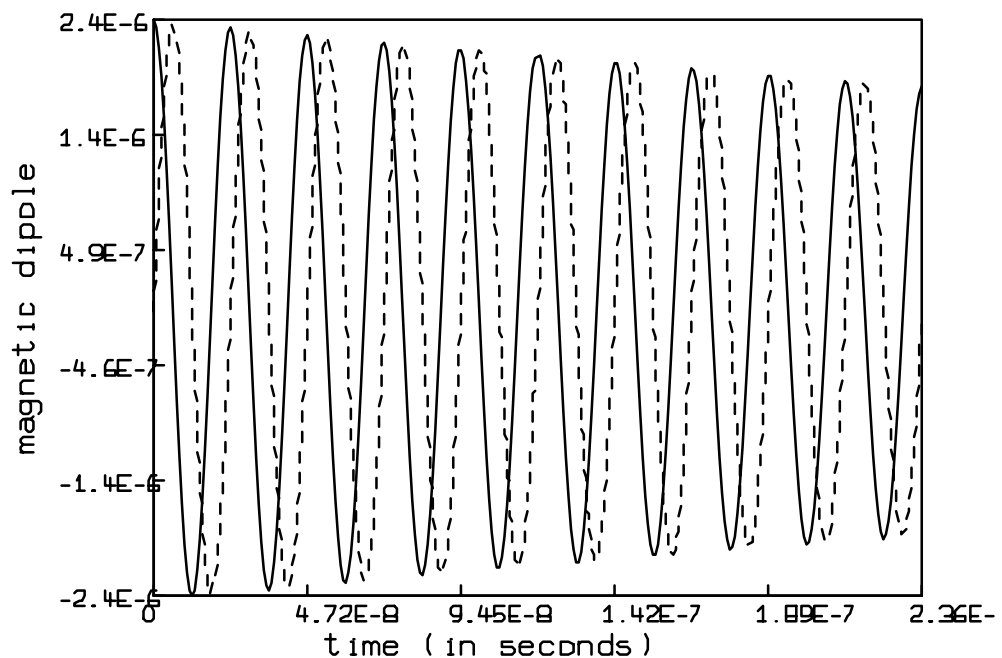
```
* unview                      /* remove the 3d picture */  
* delete w3
```

```

* btitle = "time (in seconds)"
* ltitle = "magnetic dipole"
* emfs = "delete m row 1;\
        draw t &' m col 1 lt dashed;\
        draw t &' m col 2;\
        bottom title btitle;\
        left title ltitle;"
* do emfs
* view

```

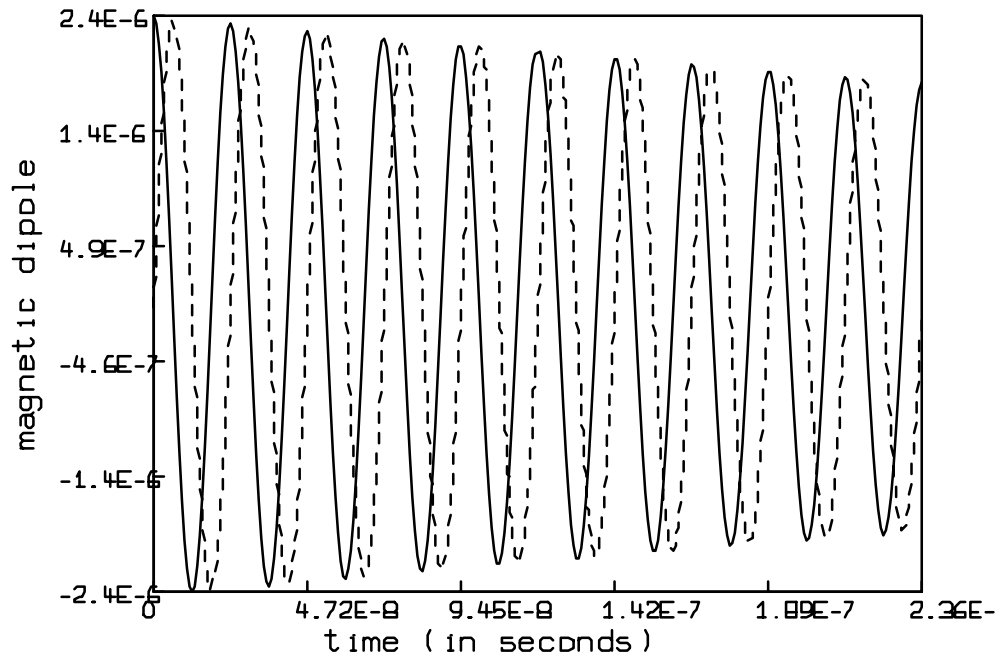
The macro `emfs` draws a graph of the x-component of the magnetic dipole versus time with a dashed line and the y-component of the magnetic dipole versus time with a solid line. It also places titles on the bottom and left axes. The following picture is then seen on the display:



The reduction in amplitude of the oscillations is characteristic of the spin-spin relaxation time, T_2 .

With the macros `pulse1`, `mdip`, and `emfs` defined above, it is a simple matter to change the relaxation constants, the pulse's angle of rotation, the strength and direction of the external magnetic field, or the gyromagnetic ratio and run the single pulse experiment again. For example, suppose the spin-spin relaxation constant, T_2 , is smaller by a factor of 10. The following commands generate the 3 dimensional perspective picture and the 2 dimensional time plot of the components of the magnetic dipole vector:

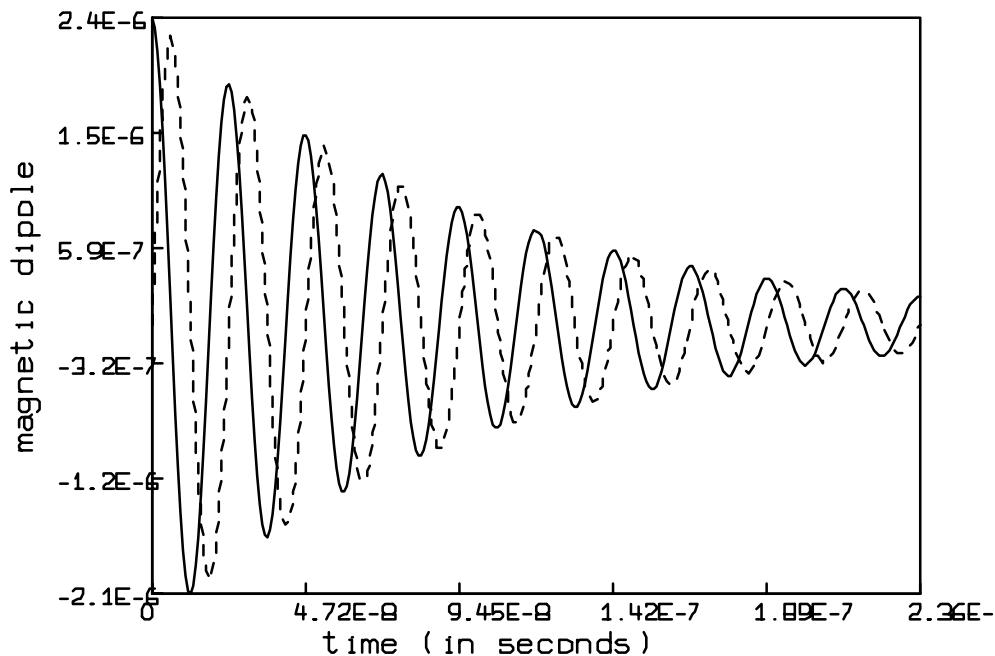
```
* unview          /* remove the previous picture */
* delete w
* t2 = 1.E-7      /* re-define the spin-spin relaxation constant */
* do pulse1       /* run the experiment */
* do mdip         /* draw the 3d picture */
* cmd3d("raise 1")
* cmd3d("truck 1")
* cmd3d("track")
* cmd3d("dolly 1")
* cmd3d("twist -20")
* cmd3d("axes")
* view
```



```

* unview          /* remove the previous picture */
* delete w3
* do emfs        /* draw the time-dependent magnetic dipole components */
* view

```



```
* unview          /* remove the previous picture */
* delete w
```

As expected, the smaller value of the spin-spin relaxation time, T_2 causes the free induction decay signal to die away faster than in the previous example.

A Double Pulse Experiment

If the external magnetic field is not homogeneous, *double* pulse experiments can be performed which give rise to resurgences of amplitude in the free induction decay signals. This effect was described by E.L. Hahn in the article “Spin Echoes” Phys. Rev. 80 (1950) 580. Here we simulate a double pulse experiment consisting of a pulse sequence in which the first pulse rotates the magnetic dipole by $\frac{\pi}{2}$ radians about the x-axis and the second pulse— τ units of time later—rotates the magnetic dipole by π radians about the x-axis. Owing to the inhomogeneities in the external magnetic field, the resurgence of amplitude in the free induction decay signal is observed τ units of time after the second pulse.

The inhomogeneity of the external magnetic field is simulated by running the pulse sequence on 10 magnetic dipoles, each subject to a different constant, external magnetic field. The Larmor frequency of precession is different for each magnetic dipole. The spin echo is then observed in the *net* magnetic dipole obtained by summing the time dependent free induction decay signals from each of the magnetic dipoles.

First we show the free induction decay resulting from the pulse sequence applied to a magnetic dipole in a *homogeneous* magnetic field. The macro `pulse1` from the previous section can be used to generate the time evolution of the magnetic dipole from the moment of the first pulse to the moment before the second pulse. We define a vector of times `tt` which holds times for the rest of the experiment.

```
* tt = tau:(2.5*tau)!(1.5*nsteps)
```

This statement assigns `tt` the values `tau` to `2.5*tau` in 450 steps. Then we define a new macro, `pulse2`, which determines the effect of the second pulse.

```
* pulse2 = "initial mx(tau) = m[nsteps,2];\  
            initial my(tau) = m[nsteps,3]*cos(beta2)+m[nsteps,4]*sin(beta2);\  
            initial mz(tau) = -m[nsteps,3]*sin(beta2)+m[nsteps,4]*cos(beta2);\  
            m = m&points(mx,my,mz,tt);"
```

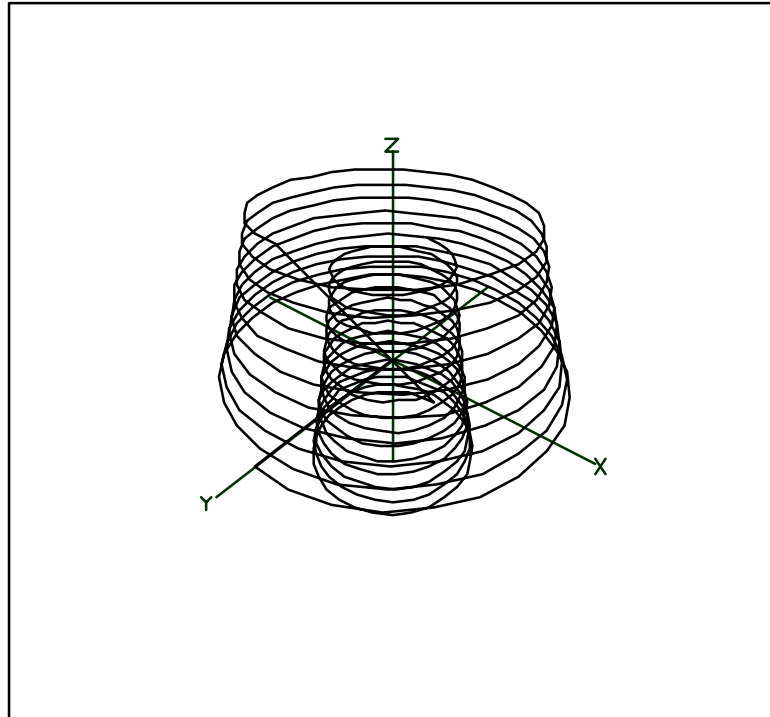
The `initial` statements in this macro find the components of the magnetic dipole at time `tau` after the second pulse has rotated the magnetic dipole about the x axis by an angle `beta2`. The `points` operator in the fourth statement solves Bloch's equations for the times in the vector `tt` and the ampersand operator concatenates the four column solution matrix from the `points` operator to the existing matrix `m` where the time evolution of the magnetic dipole from 0 to `tau` has been stored.

The following MLAB commands perform the complete double pulse sequence on a magnetic dipole in a 10000 Gauss homogeneous magnetic field:

```
* beta1 = pi/2  
* beta2 = pi  
* t2 = 5.E-7  
* do pulse1  
* do pulse2
```

To see the time evolution of the magnetic dipole in a 3 dimensional perspective, type:

```
* do mdip
* cmd3d("raise 1")
* cmd3d("truck 1")
* cmd3d("track")
* cmd3d("dolly 1")
* cmd3d("twist -20")
* cmd3d("axes")
* view
```

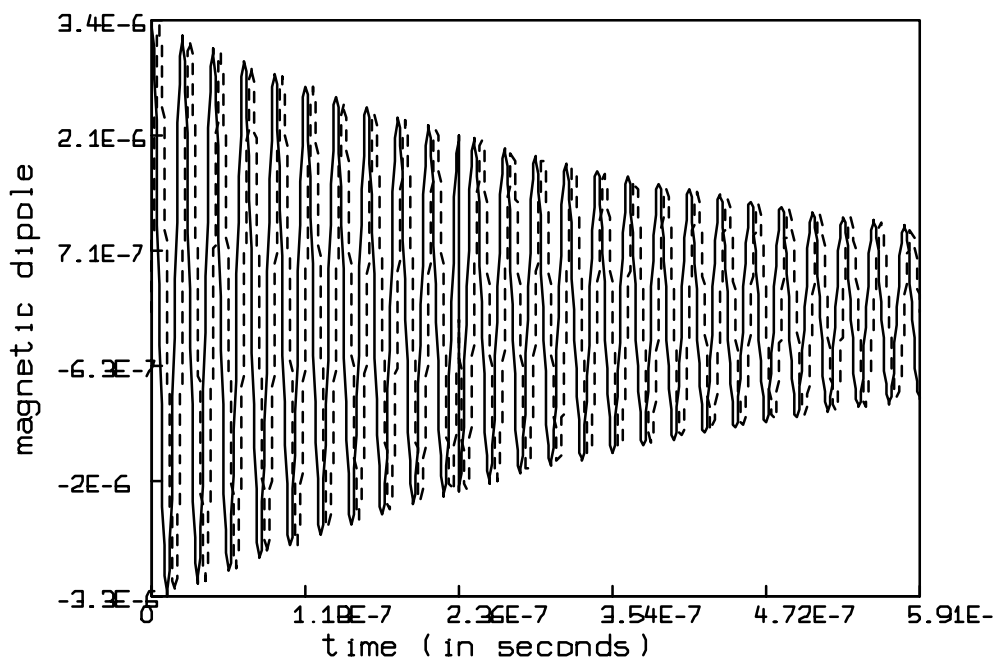


This figure shows the evolution of the magnetic dipole in a homogeneous magnetic field through the double pulse sequence. The magnetic dipole after the first $\frac{\pi}{2}$ pulse is seen as a line segment along the positive y-axis. As time progresses, the magnetic dipole precesses around the z-axis until the moment of the second pulse at time τ . When the second pulse is applied at time τ , the y and z components of the magnetic dipole are reversed. The magnetic dipole then continues to precess about the z axis, returning to its equilibrium configuration. Throughout the entire process, the magnitude of

the transverse component of the magnetic dipole is seen to decrease at a rate proportional to the spin-spin relaxation constant, T_2 .

The x and y components of the magnetic dipole, which are proportional to the free induction decay signals, are shown by the commands

```
* unview
* delete w3
* ttt = t
* t = t & tt
* do emfs
* view
```



This figure shows that in the homogeneous magnetic field, the x and y components of the magnetic dipole and, therefore, the free induction decay signals, simply die off with a characteristic time constant of T_2 . There is a change in phase of the signal when the second pulse occurs at t equals $2.36E-7$ seconds.

```

* unview
* delete w
* t = ttt

```

To demonstrate the spin echo effect, we determine the time evolution of the average of 10 distinct magnetic dipoles—each evolving in a different magnetic field. This is accomplished with the following commands:

```

* h00 = 9600:10400!10      /* the different magnetic fields */
* netp = shape(750,3,0^^2250);
* for i = 1:10 do {
>   h0 = h00[i]
>   do pulse1
>   do pulse2
>   delete m col 1
>   netp = netp+m
> }

```

First we set `h00` to be a vector of magnetic field strengths ranging in value from 9600 Gauss to 10400 Gauss in 10 steps. Actual inhomogeneities in the external magnetic field are on the order of .01 Gauss. Here, the inhomogeneity in the 10000 Gauss external magnetic field is greatly exaggerated so that the spin echo effect can be demonstrated in a short time interval.

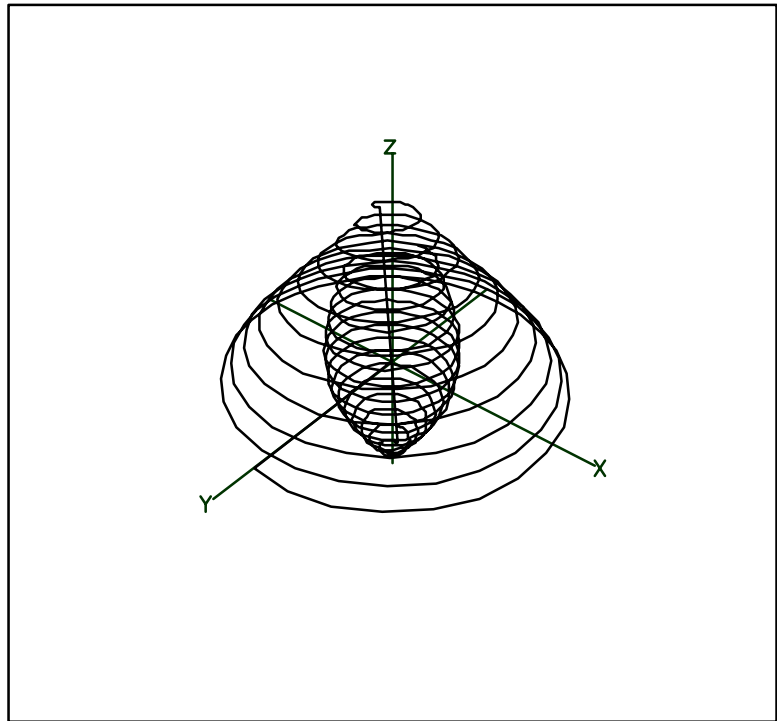
The `shape` operator is then used to initialize the 750 row by 3 column matrix `netp` to zero. The `for...do` loop runs the double pulse experiment ten times. Each time, the magnetic field is different and the time evolution of the magnetic dipole computed in `m` is accumulated in the array `netp`.

The 3 dimensional perspective view of the evolution of the net magnetic dipole is shown by the following commands:

```

* netp = (0^^'3)&netp
* draw netp lt sequence
* cmd3d("raise 1")
* cmd3d("truck 1")
* cmd3d("track")
* cmd3d("dolly 1")
* cmd3d("twist -20")
* cmd3d("axes")
* view

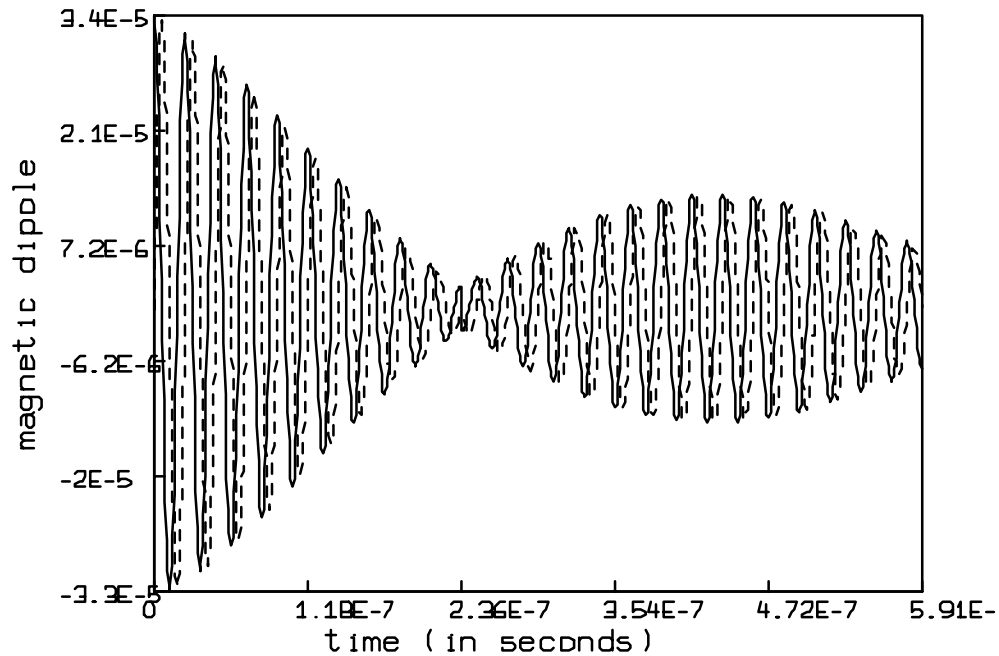
```



This figure shows that the net magnetic dipole lies along the y-axis at time 0 after the first $\frac{\pi}{2}$ pulse. The net magnetic dipole then precesses around the z-axis. The transverse component of the net magnetic dipole is seen to decrease *faster* than the magnetic dipole in the homogeneous magnetic field experiment, owing to destructive interference between the constituent magnetic dipoles precessing at different Larmor frequencies. Immediately after the second pulse, the y and z components of the net magnetic dipole are reversed. As the net magnetic dipole precesses about the z axis during subsequent evolution, there is a temporary increase in the amplitude of the transverse component of the net magnetic dipole. This is the spin echo. It is more readily seen in graphs of the x and y components of the net magnetic dipole.

```
* unview  
* delete w3  
* delete netp row 1  
* draw (t & tt) &' netp col 1 lt dashed
```

```
* draw (t & tt) &' netp col 2
* bottom title btitle
* left title ltitle
* view
```



```
* unview
* delete w
```

Conclusion

This paper has demonstrated how MLAB can be used to explore a specific differential equation model: Bloch's equations for a magnetic dipole in an external magnetic field. MLAB contains a large collection of functions, including Fourier transforms, non-linear optimization, curve fitting, statistical distribution functions and their inverses, and orthogonal polynomials.

Further information about MLAB is available from:

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