```
% Field-sweep NMR experiment on a two-spin system.
%
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function hello_world()

% Pauli matrices for spin 1/2
sigma_x=[0 1/2; 1/2 0];
sigma_y=[0 -1i/2; 1i/2 0];
sigma_z=[1/2 0; 0 -1/2];
unit=[1 0; 0 1];

% Two-spin operators
Lx=kron(sigma_x,unit); Ly=kron(sigma_y,unit); Lz=kron(sigma_z,unit);
Sx=kron(unit,sigma_x); Sy=kron(unit,sigma_y); Sz=kron(unit,sigma_z);

% Create the Hamiltonian superoperator
H=2*pi*100*Lz+2*pi*200*Sz+pi*20*(Lx*Sx+Ly*Sy+Lz*Sz);
H=kron(eye(size(H)),H)-kron(transpose(H),eye(size(H)));

% Reaxation superoperator
R=-2.0*eye(16,16);

% Equilibrium state
rho_eq=Lz(:)+Sz(:);

% Perturbation operator
P=2*pi*0.1*(Lx+Sx);
P=kron(eye(size(P)),P)-kron(transpose(P),eye(size(P)));

% Sweep operator
S=Lz+Sz;
S=kron(eye(size(S)),S)-kron(transpose(S),eye(size(S)));

% Observables
obs1=Lx(:)+Sx(:); obs2=Ly(:)+Sy(:); obs3=Lz(:)+Sz(:);

% Experimental parameters
npoints=10000;

% Pre-allocate the answers
answer1=zeros(npoints,1); answer2=zeros(npoints,1); answer3=zeros(npoints,1);

% Set sweep range
sweep_range=linspace(0,300,npoints);

% Do the simulation
parfor n=1:numel(sweep_range)

    % Add magnet sweep terms
    current_H=H-2*pi*sweep_range(n)*S+P;

    % Get inverse-times-vector
    sigma=(-1i*current_H+R)\(R*rho_eq);
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```
    % Compute the answers
    answer1(n)=obs1'*sigma;
    answer2(n)=obs2'*sigma;
    answer3(n)=obs3'*sigma;

end

% Plotting
subplot(3,1,1); plot(-real(answer1));
subplot(3,1,2); plot(-real(answer2));
subplot(3,1,3); plot(real(answer3));

end
```

```
%Mem=2GB
%NProcShared=4
%Chk=geometry.chk
#p opt=tight b3lyp/cc-pVDZ
   scf=tight integral=(grid=ultrafine)

Gaussian input for geometry optimization

0 1
 C                  0.07798700    0.03646600    0.00264600
 C                  1.30793300    0.55172400   -0.02038900
 H                  1.45955100    1.62273600   -0.05022900
 H                  2.16813000   -0.10112000    0.01988600
 F                 -0.10495200   -1.30171100    0.00288000
 N                 -1.14596200    0.68073400    0.09226800
 H                 -1.10004900    1.67378300   -0.09304000
 H                 -1.87684700    0.22572000   -0.44195700
```

```
%Mem=2GB
%NProcShared=4
%Chk=geometry.chk
#p nmr=(giao,spinspin,mixed) b3lyp/cc-pVTZ scf=tight
   output=pickett integral=(grid=ultrafine)

Gaussian input for magnetic properties calculation

0 1
 C                  0.07799100   -0.03646700   -0.00264800
 C                  1.30789500   -0.55177600    0.02038600
 H                  1.45940600   -1.62280900    0.05019500
 H                  2.16815000    0.10099100   -0.01980000
 F                 -0.10488900    1.30172200   -0.00291500
 N                 -1.14598500   -0.68069300   -0.09223400
 H                 -1.10013400   -1.67374100    0.09305900
 H                 -1.87683700   -0.22562900    0.44198900
```