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MATLAB Graphical User Interface for Product Operator Formalism of Spin-1/2 for Nuclear Magnetic Resonance

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Purpose

This program is designed to handle the product operator formalism of spin-1/2 nuclei for Nuclear Magnetic Resonance (NMR) using MATLAB Graphical User Interface (GUI). The GUI is designed with high flexibility. The program will be helpful for educational use, for example, showing how to calculate product operators and explaining how pulse sequence components, such as Hahn-echo, INEPT etc., work.

Requirements

This program uses a MATLAB module to calculate product operators. The module is available at https://github.com/ohgo1977/ProductOperator. MATLAB and MATLAB Symbolic Math Toolbox are required for this module.

How to Use Program

Setting Path for Program

All required files are included in the folder PO_GUI_Matlab. Add this folder to your MATLAB path so that the program can be called from any working directory.

How to Launch GUI window

From the Command Window, type in

```
>> PO_GUI
```

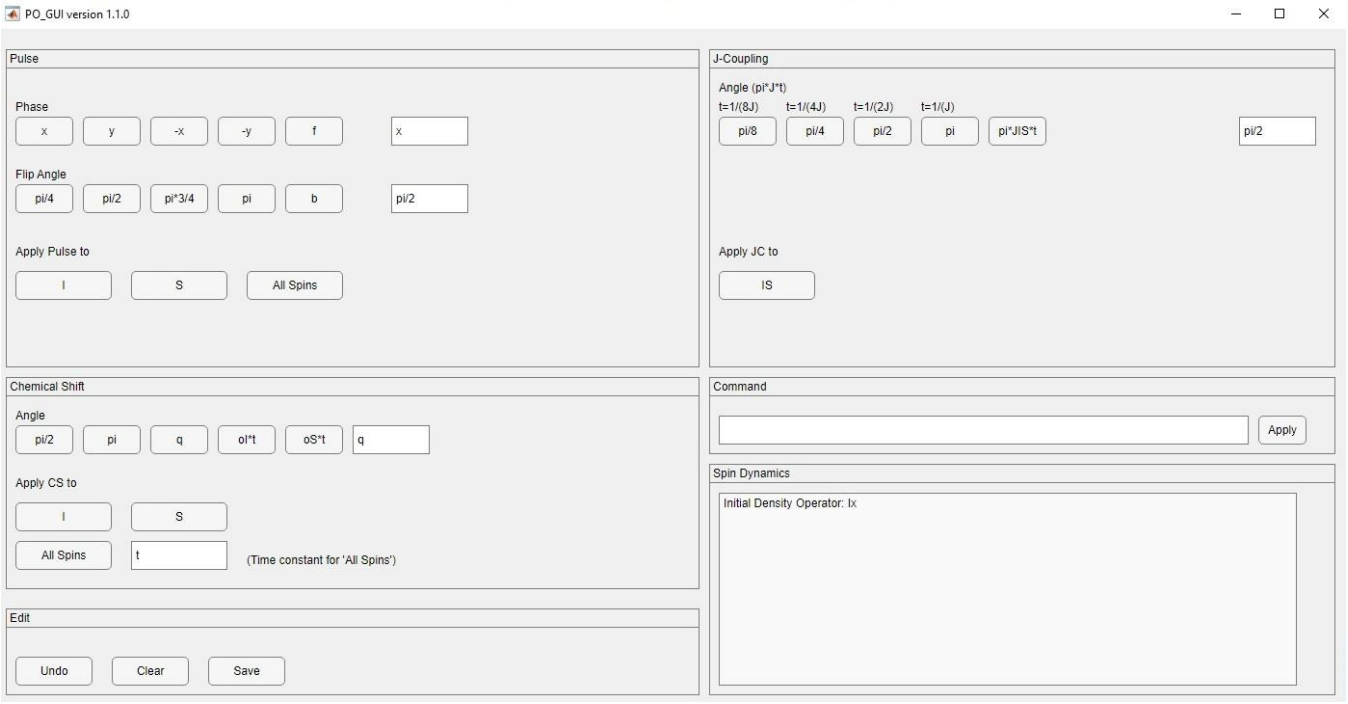
Initial Setup

Two questions will appear in the Command Window for the initial setup.

```
Enter Spin Labels Separated by Commas (Default: I,S):
Enter Initial Density Operator (Default: Iz + Sz):
```

The first question is the labels of spins you like to use. For example, if you like to create a 3-spin system with labels [I1, I2, I3], input I1,I2,I3. The default value is I,S for the I-S spin system. The GUI can display up to 5 spins. The second question is the initial density operator. You can use arbitrary coefficients with the spin operators, e.g., ai*Ix*cos(qi). The default value is a sum of z-operators generated automatically from the spin labels (e.g., Iz + Sz for I-S spin system).

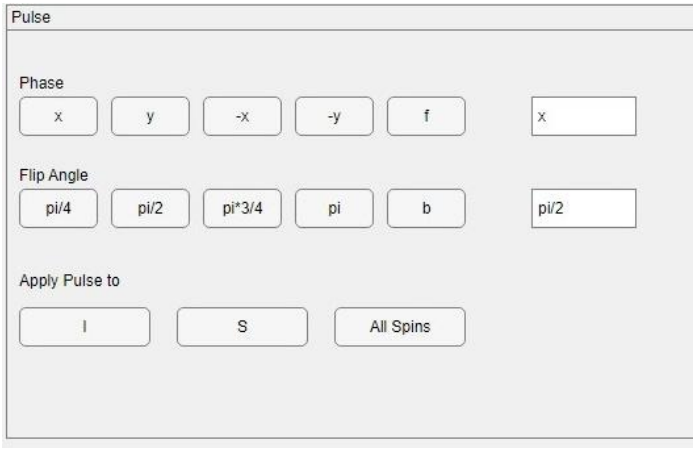
Then, the GUI window appears.



The figure above is the case of the I-S spin system with Ix as an initial density operator.

Pulse Frame

The GUI for the pulse is shown below.



1st row: Phase

You can select a phase from the quadrature phases, a phase ‘f’, or arbitrary phase that can be typed in.

2nd row: Flip Angle

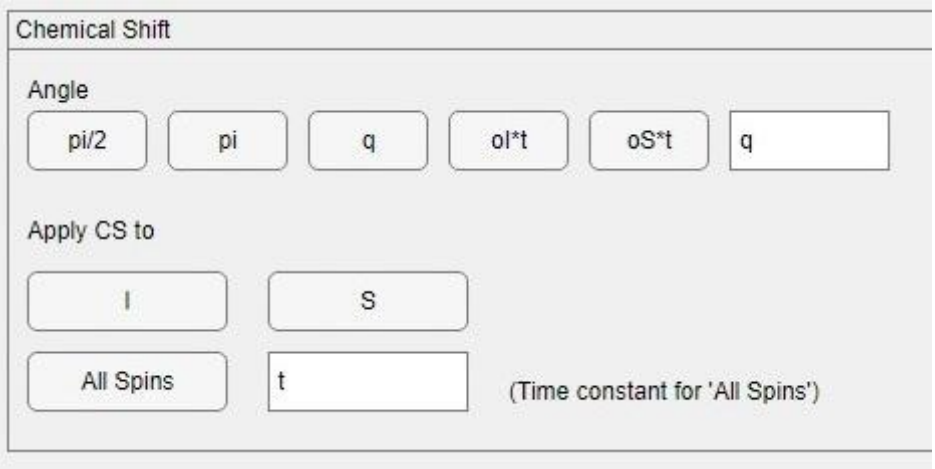
You can select a flip angle from pi/4, pi/2, pi*3/4, pi, an angle ‘b’, or arbitrary angle that can be typed in.

3rd row: Spin Type

You can apply a pulse with the selected phase and flip angle to one of the spins or all spins.

Chemical Shift Frame

The GUI for the chemical shift is shown below.



1st row: Angle

You can select an angle of the chemical shift evolution from pi/2, pi, ‘q’, ‘oI*t’, ‘oS*t’, or arbitrary angle that can be typed in. Note that ‘I’ and ‘S’ in ‘oI’ and ‘oS’ are automatically labeled from the spin labels.

2nd row: Spin Type

You can select a spin type for the chemical shift evolution with the angle selected. If the ‘All Spins’ button is pushed, angles corresponding to all spins are generated with a time constant in the input window. For example, if the spins are ‘I’ and ‘S’ with a time constant ‘t’, the angles are ‘oI*t’ and ‘oS*t’. Another example is that the angles ‘oI1*t1’, ‘oI2*t1’, and ‘oS3*t1’ for the spins ‘I1’, ‘I2’, and ‘S3’ with a time constant ‘t1’.

***J*-coupling Frame**

The GUI for the *J*-coupling is shown below.

1st row: Angle

You can select an angle of the *J*-coupling evolution from pi/8, pi/4, pi/2, pi, 'pi*JIS*t' or arbitrary angle that can be typed in. Note that 'IS' in 'JIS' is automatically labeled from the spin labels.

2nd row: Spin-pair Type

You can select a pair of spins for the *J*-coupling evolution with the angle selected.

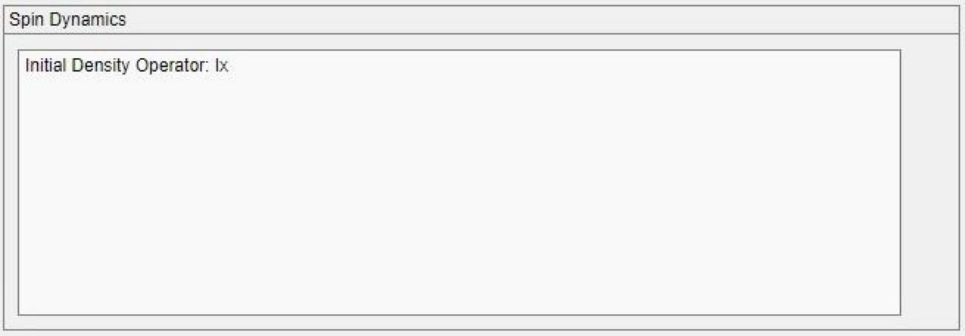
Command Frame

You can type in and execute a PO module command from the GUI below.

A command line in the text window will be executed by pushing the 'Apply' button. The command should have a form without including a PO object. For example, `pulse({'I'},{'x'},{q})` not `rho.pulse({'I'},{'x'},{q})` nor `pulse(rho, {'I'},{'x'},{q})` where rho is a PO object. Details are in the manual of the PO module.

Spin Dynamics Frame

The result of the calculation is shown in the text frame. A slide will appear once the results don't fix in the frame.



Edit Frame

The GUI for editing is shown below.

‘Undo’ Button

You can undo the process with this button.

‘Clear’ Button

You can start the process from the initial state you type in.

‘Save’ Button

You can save the text in the text box to a text file. A dialog will appear for saving.

Examples

Hahn-echo in 1-spin system

In this example, the initial density operator Iz becomes Ix by a $\pi/2_y$ pulse followed by the chemical shift evolution. Then, a π_x pulse is applied. After the second chemical shift evolution, the density operator becomes Ix again, meaning that the chemical shift is refocused.

```
Initial Density Operator: Iz
Pulse: I  90y
   Ix
CS: I q
   Ix*cos(q) + Iy*sin(q)
Pulse: I 180x
   Ix*cos(q) - Iy*sin(q)
CS: I q
   Ix
```

Spin-echo in 2-spin system for *J*-decoupling

In this example, the magnetization Ix evolves under the chemical shift and *J*-coupling. Then a π-pulse is applied to the S-spin. After the second period of chemical shift and *J*-coupling, only the chemical shift evolves with the angle of 2*oI*t.

```
Initial Density Operator: Ix
CS: I oI*t
   Ix*cos(oI*t) + Iy*sin(oI*t)
JC: IS JIS*t*pi
    - 2IxSz*sin(oI*t)*sin(JIS*t*pi) + Ix*cos(oI*t)*cos(JIS*t*pi) +
2IySz*cos(oI*t)*sin(JIS*t*pi) + Iy*sin(oI*t)*cos(JIS*t*pi)
```

```
Pulse: S 180x
   2IxSz*sin(oI*t)*sin(JIS*t*pi) + Ix*cos(oI*t)*cos(JIS*t*pi) -
2IySz*cos(oI*t)*sin(JIS*t*pi) + Iy*sin(oI*t)*cos(JIS*t*pi)
CS: I oI*t
   2IxSz*2*cos(oI*t)*sin(oI*t)*sin(JIS*t*pi) + Ix*cos(2*oI*t)*cos(JIS*t*pi) -
2IySz*cos(2*oI*t)*sin(JIS*t*pi) + Iy*2*cos(oI*t)*sin(oI*t)*cos(JIS*t*pi)
JC: IS JIS*t*pi
   Ix*cos(2*oI*t) + Iy*sin(2*oI*t)
```

References

Levitt, M. H., *Spin Dynamics*, 2nd Edition, Wiley, **2008**.

Keeler, J., *Understanding NMR Spectroscopy*, 1st Edition, Wiley, **2005**.

Hassan, J., Nabulsi, A. A., *A New Graphical User Interface for Teaching NMR*, *Am. J. Edu. Res.*, **2014**, *2*, 240-244.

Brown, K. C., *wXprodOp A Product Operator Calculator*, **2017**.

https://sourceforge.net/projects/wxprodop/

http://nmrwiki.org/wiki/index.php?title=Product_operator_calculator_-_wxProdOp