The Magpie manual

Wouter Franssen & Bas van Meerten

Version 0.0

18th July 2022

Contents

1 Introduction

Magpie (waar staat het voor?) is a program that simualtes an NMR spectrometer environment. It can load sample and pulse sequences, and simulate the outcome of NMR measurements. The goal of the program is to be used in teaching, allowing students a first introduction to practical NMR.

2 Running Magpie

2.1 Python and library versions

Magpie should run on python versions starting from 3.8. For the library version, the following are needed:

- `numpy` >= 1.23.1
- `matplotlib` >= 3.5.2
- `scipy` >= 1.8.1

- PyQt5 >= 5.15.7

Older library and python version might also work, but have not been tested.

2.2 Installing

2.2.1 Linux

On Linux, Magpie can be most efficiently run using the python libraries that are in the repositories. For Ubuntu, these can be installed by running:

```
sudo apt install python3 python3-numpy python3-matplotlib python3-scipy
python3-pyqt5
```

Navigating to the `magpie/src` directory in a terminal, Magpie can then be run by executing `python3 magpie.py`.

2.2.2 Windows

On Windows, the relevant python libraries can be installed by installing `anaconda`: https://www.anaconda.com/download/. If you do not have another python version installed already, make sure to add anaconda to the `path` during the install. In this case, Magpie can be run by executing the `WindowsRun.bat` file in the `magpie/src` directory.

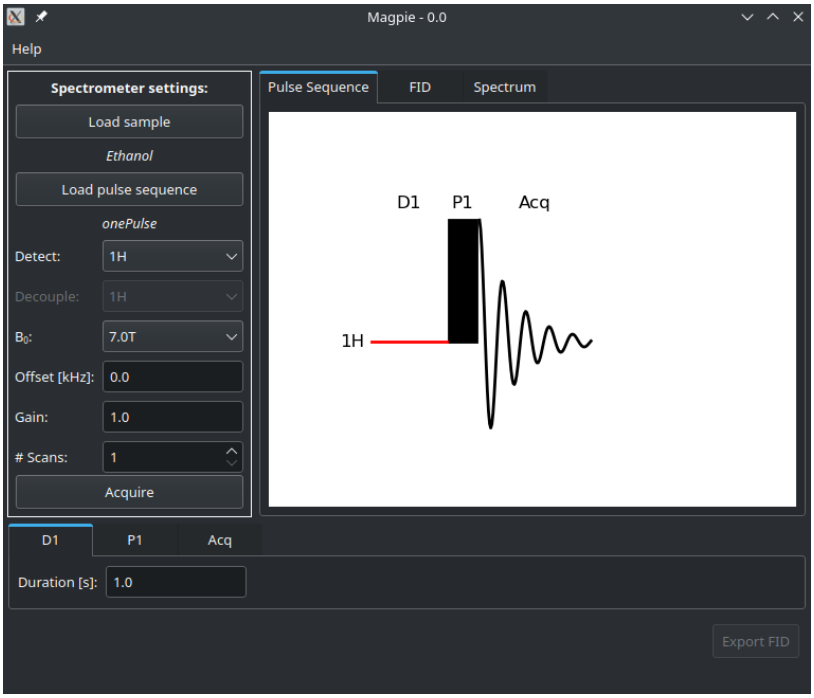
If you already have other version of python installed, adding anaconda to the `path` might create issues. Do not do this in this case. When not added to the path, the `WindowsRun.bat` should be edited in such a way that `pythonw` is replaced with the path to your `pythonw.exe` executable in the anaconda install directory.

2.2.3 OS X

On OS X, the relevant python libraries can be installed by installing `anaconda`: https://www.anaconda.com/download/. Navigating to the `magpie/src` directory in a terminal, Magpie can then be run by `anacondapython magpie.py`, with `anacondapython` replaced by the path to your anaconda python executable.

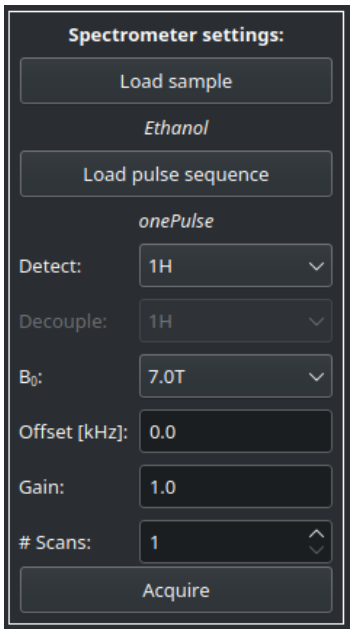
3 Interface

The Magpie interface looks like this:



In the sections below, the individual elements are explained.

3.1 Spectrometer settings

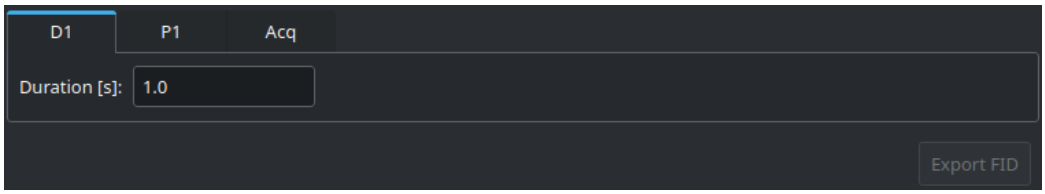


In the left of the Magpie screen, the spectrometer settings can be put in. These are all settings that are not specific to a pulse sequence. Also, the buttons to load a sample and a pulse sequence are contained here. Below is a list of the settings and their description.

- **Load sample:** Opens a file dialog to brows for a sample file. More info can be found in section 4. The file should have extension `.txt`.

- **Load pulse sequence:** Opens a file dialog to brows for a pulse sequence file file. More info can be found in section 5. The file should have extension `.csv`.
- **Detect:** The nucleus to detect. In principle, any nucleus can be detected. For the moment, we limit the selection to ^{1}H and ^{13}C though. This is a design choice to not overflow the user with obscure nuclei.
- **Decouple:** The nucleus that is decoupled during a decoupling pulse sequence element. Only active if the pulse sequence has a decouple element.
- **B_0:** The main magnetic field strength in Tesla. Magpie supports any magnetic field strength. For now, we decide on using a dropdown box with only common fields. This is the teach the user that in reality the magnetic field cannot easily be changed to whatever we want.
- **Offset [kHz]:** The transmitter offset in kHz. This can be used to fine-tune the center frequency of the experiment. It defines the center of the spectrum, as well as the frequecy on which any pulses are given.
- **Gain:** The gain factor of the receiver. All signals are multiplied by this value before detection. Note that, contrary to most real-life spectrometers, Magpie uses a linear scale, and does not work in dB.
- **# Scans:** The number of individual scans that need to be recorded. All scans are automatically summed.

3.2 Pulse sequence settings

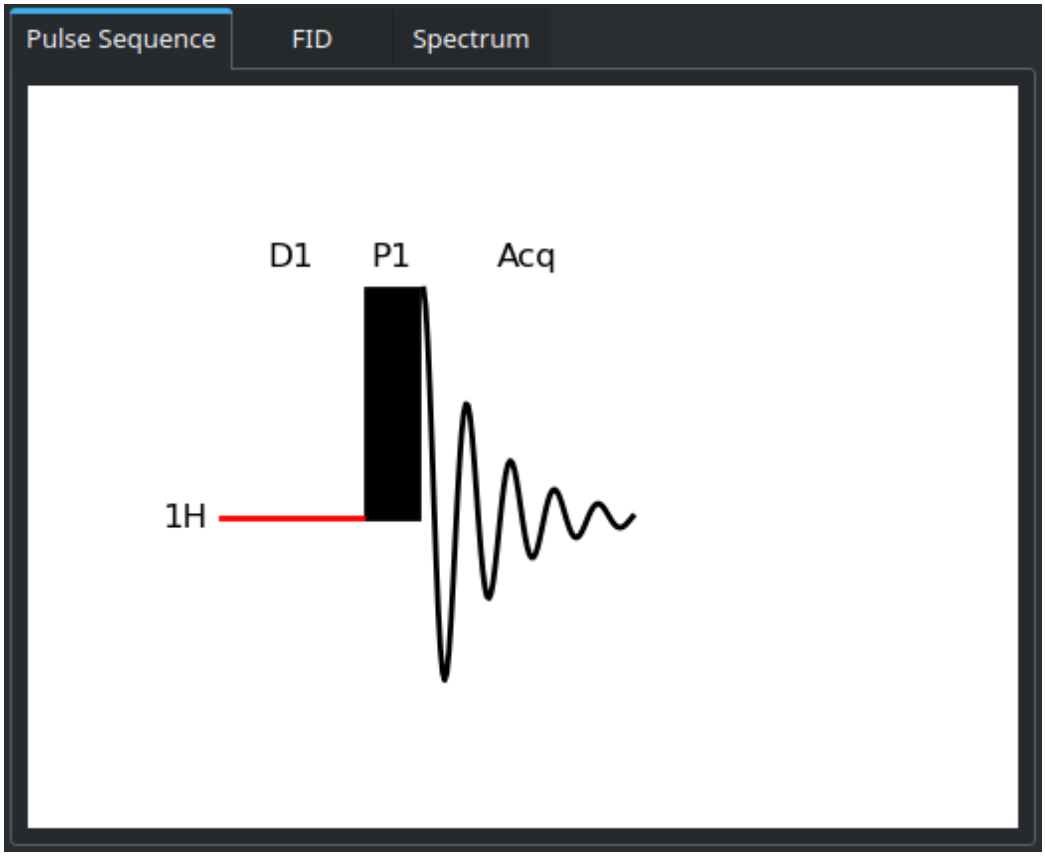


In the bottom of the Magpie interface, the pulse sequence settings are defined. Each tab represent a separate element of the pulse sequence. The names of the tabs are equal to the names of the elements, as defined in the pulse sequence file. The pulse sequence diagram (in the plot window) always highlights the element which settings tab is currently showing. More info on pulse sequences, and the relevant settings per element can be found in section 5.

3.3 Plot windows

The plot window contains three tabs: Pulse sequence, FID, and Spectrum. These are explained below.

3.3.1 Pulse sequence

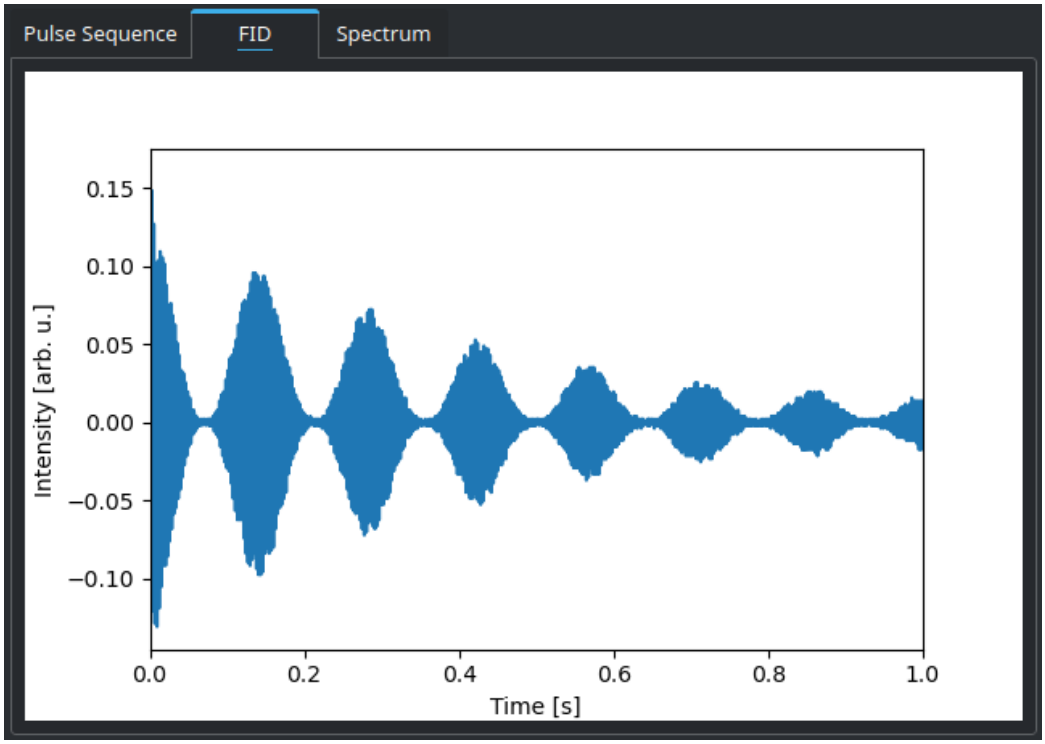


The pulse sequence tab displays a diagram of the current pulse sequence. The current element that is selected is displayed in red. Left-clicking on an element changes the selection. The sequence settings tab (see subsection 3.2) folows this selection (and vice-versa).

The labels displayed above the sequence elements are those as defined in the pulse sequence file. The tabs in the sequence settings window also have this name.

The elements in the pulse sequence each have a unique pictorial representation. The style of the elements is not updated depending on the pulse sequence settings (e.g. a pulse with amplitude 0 is not shown as a much lower rectangle).

3.3.2 FID

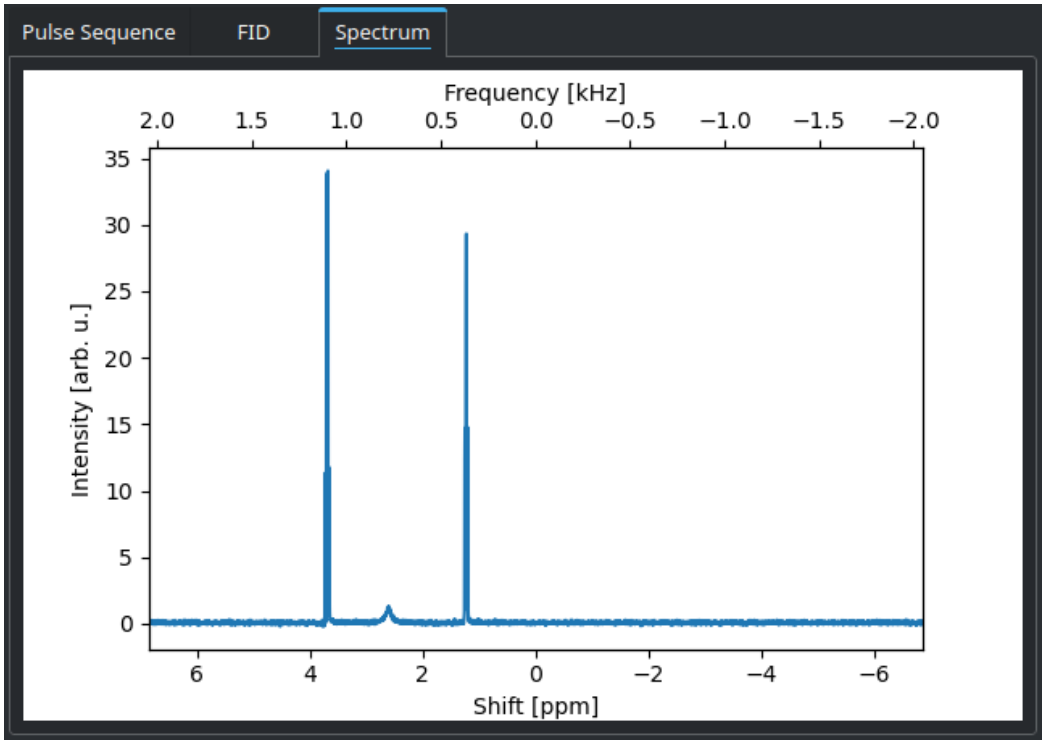


The FID tab shows the FID (time signal) of the simulated data. If there is no data, no plot is shown. The y-axis has the signal intensity. Although it is in arbitrary units, the maximum value is 1. Any signals high than that will be rounded to 1. For negative intensity the limit is −1. These situations relate the 'receiver overflow' in real spectrometers, that happens when signals are to strong to properly digitize.

The plot supports the following mouse-based zoom-controls:

- Dragging a box while holding the left mouse button creates a zoombox, and will zoom to that region.
- Dragging while holding the right mouse button drags (i.e. pans) the spectrum. Doing this while holding the Control button pans only the x-axis, holding Shift pans only the y-axis.
- Double clicking with the right mouse button resets the view to fit the whole plot (both x and y).
- Scrolling with the mouse wheel zooms the y-axis. Doing this while also holding the right mouse button zooms the x-axis. By holding Control the zooming will use a larger step size.

3.3.3 Spectrum



The Spectrum tab shows the signal after Fourier transformation. Two x-axes are plots:

- Bottom x-axis: Has the axis in ppm. Here, 0 ppm relates to the signal of the ppm reference for the measured nucleus. If the spectrometer offset is changes, the 0 ppm position can shift in the spectrum.
- Top x-axis: Has the axis in kHz. For this axis, 0 kHz is always defined in the center of the spectrum. When adjusting the spectrometer offset, this axis can be used to find the desired shift.

The spectrum plots has the same zoom controls as the FID plot (see subsubsection 3.3.2).

4 Sample definition

Sample files for Magpie need to be in a specific definition. They need to be text files with `.txt` extension.

The file should start with a header:

```
###SAMPLE###
```

Below this, on optional statement regarding the sample amount (concentration) can be made:

```
amount 1
```

In this case, the scaling is set to 1, so it has no effect.

After this, a molecule can be defined. The sample file can hold multiple molecule definitions. Within this block, the spins are set, as well as the overall relaxation times and the J-couplings.

The statements are:

Statement	Input	Description
amount	amount	molecule amount
T1	T1	Overall T1, in seconds (optional)
T2	T2	Overall T2, in seconds (optional)
T2prime	T2prime	Overall T2prime, in seconds (optional)
spin	isotope shift multiplicity	For example: 1H 1.2 3
spin	isotope shift multiplicity T1 T2 T2prime	Spin definition including relation times. These are used in favour of the overall relaxation times, if set. Values can be set empty by an underscore (_)
J	spin1 spin2 strength	Set J-coupling in Hz between two spin indexes. Number order as the spins are defined. For example: J 1 2 9.6
Jmatrix	matrix	Set J-coupling in Hz between all spins in matrix format. Example for two spins: [[0,10],[10,0]], setting 10 Hz coupling. Size needs to be n_spins x n_spins. When used the, regular J statement cannot be used.
pair	isotope shift1 shift2 k amp1 amp2 T1_1 T1_2 T2_1 T2_2	Sets a spin-pair with exchange between them. amp sets the multiplicity. Individual T1 and T2 times can be set, or set to empty by an underscore (_). No J-couplings can be set to these spins.

Either Jmatrix or J statements are allowed. Not both. Spin statements can lack all the relaxation times, or have a _ instead. If a relax time not defined for a spin, it needs to use the global molecule relaxation time. These are also optional, but if they lack, the individual spin lifetimes need to be all there.

An example definition could be the following sample:

```
###SAMPLE###
amount 1
```

```
###MOLECULE###
amount 0.1
T1 5
T2 0.5
T2prime 10
spin 1H 1.2 3
spin 1H 3.6 2
J 1 2 7
```

Here we set a two spin system, with shifts 1.2 and 3.6 ppm, multiplicities 3 and 2. There is a 7 Hz J-coupling between the spins. All nuclei have the same relaxation times, set at 5, 0.5 and 10 s for T1, T2 and T2prime respectively. The overall intensity scaling is set at 1, and the molecule itself has scaling 0.1.

A more complicated sample could be ethanol:

```
###SAMPLE###
amount 1
###MOLECULE###
amount 0.98
T1 5
T2 0.5
T2prime 10
spin 1H 1.226 3
spin 1H 3.692 2
spin 1H 2.605 1 _ 0.01 0.1
J 1 2 7
###MOLECULE###
amount 0.01
T1 5
T2 1
T2prime 10
spin 1H 1.224 3
spin 1H 3.692 2
spin 1H 2.605 1 _ 0.01 0.1
spin 13C 18.1 1 _ _ 7
J 1 2 7
J 1 4 125
###MOLECULE###
amount 0.01
T1 7
T2 1
```

```
T2prime 10
spin 1H 1.226 3
spin 1H 3.692 2
spin 1H 2.605 1 _ 0.01 0.1
spin 13C 57.8 1 _ _ 7
J 1 2 7
J 2 4 125
```

Here we set three molecules: with no 13C nucleus, and both options with a single 13C nucleus (the 13C-13C variant is too low in intensity to care about). The amount of the molecules is set to follow the natural abundance. For the OH peak (at 2.6 ppm), a separate set of relaxation times is set, as to have a shorter T2 and T2prime, to include the fact that this signal is usually exchanging causing line broadening. J-couplings are ste between the 1H nuclei of the CH_3 and CH_2 groups, as well as between the 13C nuclei and their directly bonded 1H nuclei.

5 Pulse sequence definition

6 Data output

7 Simulation background

Magpie uses a classical simulator, so no quantum effects are included. J-couplings are therefore included only as their weak coupling limit, and no coherence between the J-states exists.

8 Contact

To contact the `magpie` team write to `ssnake@science.ru.nl`.