

TNMR Frappy-NICOS Integration

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1 Introduction

This document is meant to outline how one can set up a TNMR-frappy server, as well as a NICOS-frappy connection, and some basic information to understand the details "under the hood." Further, it provides limited technical details (i.e., programming reference); the majority of these details should be outlined in the Programming Guide¹ or in-line comments.

¹https://forge.frm2.tum.de/public/doc/frappy/html/

2 TNMR Interfacing

Tecmag's TNMR software does not have an official API, but it does come shipped with a Component Object Model (COM)² interface. This is intended as a means of scripting small experiments inside the TNMR interface, so there are limitations to the interfacing possibilities. Despite this, an API and helper library was written in Python to provide core functionalities, including:

- Pulse sequence generation
- Pulse sequence file generation
- Live parameter alteration
- Data acquisition starting, aborting
- File loading/saving

This API and library are typically hidden from the NICOS user within the Frappy server code, but the passionate user is welcome to contribute³.

The Frappy server directly connects to an instance of TNMR if one is found, via the COM interface as described above. You will see errors if it cannot find an open instance of the program, and it should be opened at any time, before or after the Frappy server is started, but of course before attempting to take data or execute commands from NICOS.

²https://learn.microsoft.com/en-us/windows/win32/com/component-object-model--com--portal

³https://github.com/SampleEnvironment/frappy

3 Connection Scheme

In the most basic NMR experiment using this system, there is only one computer, running TNMR, a Frappy server, and a NICOS server. This is perhaps unrealistic for many institutions, as often the TNMR instance is running on a standalone system, disconnected from external devices such as cryostats and magnets. It is entirely possible, and encouraged, to separate these systems, so the TNMR instance and pulse generation and data acquisition (DAQ) hardware are connected to a dedicated PC. This is the configuration that this system was written for, so the rest of the documentation will assume it.

For notation, the PC running the TNMR instance and connected to the pulse generation and DAQ hardware will be referred to as the "NMR PC" and the system running the NICOS server will be referred to as the "control interface".

The basic pipeline for commands the user wishes to execute is as follows:

- 1. A user enables the TNMR module in NICOS on the control interface, and connects by entering the correct network address
- 2. A command is sent via NICOS on the control interface
- The loaded TNMR NICOS module leverages SECoP to send the command to the NMR PC
- 4. The NMR PC receives this command, starting the necessary processes (i.e., starting an acquisition cycle, changing parameters in TNMR, gathering data, etc.) and sending back polled values through SECoP.
- The NICOS server receives new values and updates the user display accordingly.

See Fig. 1 for a graphical outline of the connection scheme for an NMR experiment.

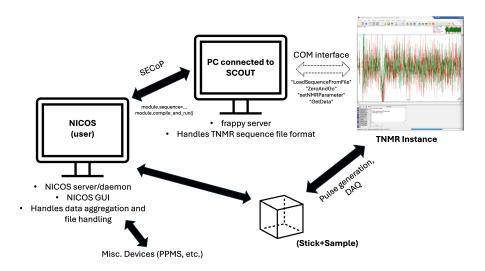


Figure 1: A connection diagram which outlines how each system in a typical NMR experimental setup should interact with each other. An instance of TNMR is open on a PC connected to a transmitter/receiver (in this case, a Tecmag SCOUT⁶), which runs a Frappy server. This Frappy server then connects to a NICOS server via SECoP⁷, and the end user interacts only with NICOS.

4 Setup

4.1 TNMR/Frappy Setup

On the TNMR PC, Frappy should be downloaded from the Git repository:

```
git clone https://github.com/SampleEnvironment/frappy
cd frappy
python -m pip install -r requirements.txt
python -m pip install pywin32 pythoncom
```

This will install Frappy, its requirements, and a Python/COM interface library. This may take some time. Further, after this is complete, it is recommended to navigate to the install location for pywin32 and run the post-install script, pywin32_postinstall.py.

Before starting an instance of the frappy server, it is important that the user navigates to frappy/frappy_psi/tnmr/templates and, if not using the SCOUT, replaces the files dashboard.txt and tmp.tnt with working dashboard and .TNT files respectively. The values in these do not matter particularly, but a working base configuration otherwise is necessary. This is due to some TNMR dodginess. It is also encouraged that the user adds their setup files to the setup_files folder, under the name of their device, to develop a small library of working setups. Who knows, perhaps setup files suitable for your device are there already?

After starting an instance of TNMR (see Tecmag's website for guidance on installation), the Frappy server should be started. In a terminal (potentially the same one as used for the above), navigate to the Frappy base directory and run the following:

```
python bin\frappy-server frappy_OTFMod
```

This will start the Frappy server, with the appropriate configuration file (configuration files are found in cfg/. In this case, the configuration used is frappy_OTFMod_cfg.py) for TNMR interaction. The user is free to write their own configuration file as well, but one is provided with core functionality for ease of use. They are quite simple to write, and there are plenty of examples to learn from, if one is documentation-averse. Once the server is started, the process of setting up the NMR PC is complete! Keep TNMR and the console used open.

Some additional considerations:

- Windows updates should be disabled, as well as they can be, to minimise interruptions.
- Intel Speed Shift and Intel Speed Step (settings in the BIOS of some Intel-based PCs) should be disabled; these have been known to cause cryptic problems which can cause lost time.
- USB Auto-Suspend and hard disc shutoff timers should be disabled to avoid similar problems.

4.2 NICOS Setup

This section does not provide a tutorial for configuring NICOS in its entirety⁸, but rather a basic setup including just a TNMR interface. Further, it assumes that NICOS is already installed and you know where!

There exists a repository⁹ with configuration files, helper function definitions, and example scripts for a basic NMR setup NICOS interface. To install these, execute the following to download the scripts from the base NICOS directory (often named nicos/, where one would find bin/, data/, and nicos_sing/):

Now there are a few tasks to be completed:

- nicos_sinq/tnmr/nicos.conf has several values to be updated: cache ports, daemon ports, filepaths, etc.
- nicos_sinq/tnmr/setups/frappy_tnmr.py contains the saved data's filename template, as well as the default address to find the TNMR PC at.

⁸https://forge.frm2.tum.de/nicos/doc/nicos-stable/installconfig/

⁹https://github.com/Davis-Garrad/NICOS-TNMR

Beyond these items, you can also adjust the GUI, filesinks, etc. if desired. This is covered under NICOS documentation, so it will not be covered here, except a listing of options that this package provides:

- HDF5 Datasink (nicos_sing/tnmr/sinks/HDF5.py)
- NeXus Datasink (nicos_sinq/tnmr/sinks/HDF5_NEXUS.py)
- Custom TNMR-purposed commands (nicos_sinq/tnmr/commands/tnmr_commands.py). This should almost certainly be included in any setup. See Sec. 6.1 for more detail.
- Demo setups (nicos_sinq/tnmr/setups)
- Example scripts (nicos_sinq/tnmr/example_scripts)

Once everything is configured as one desires, one can start the frappy server:

```
python {frappy root directory}/bin/frappy-server {cfg}
```

where {cfg} denotes a particular configuration file (as described in the frappy documentation) in cfg/. This could be, for example, psi_nmr_setup if the filename is psi_nmr_setup_cfg.py. Frappy, when starting a server, searches for files in the cfg/ folder, ending with _cfg.py. Once the frappy server is initialised, one should start the NICOS server on a Linux machine (see 7):

```
{NICOS root directory}/bin/start.sh
```

Finally, the user can open a NICOS GUI or CLI and simply connect to the server configured in the previous step. If unsure of the address to connect to, it is helpful to look at the configuration files and the output of the NICOS server start command.

4.3 Installing DNMR

While the NICOS setup provides a framework for generating NeXus files to store NMR data, there does not exist (to the author's knowledge) a suitable analysis software. While the user of this system is encouraged to write any tooling they need as they like, there does exist an easily extensible open-source project called DNMR¹⁰, built specifically for this system and purpose. This can be found either on Pip,

¹⁰https://pypi.org/project/DNMR/

```
python -m pip install DNMR
```

which should install all necessary dependencies. If the user is more concerned with the inner workings of the software and/or wants to extend upon it, the source can also be found at its public GitHub repository,

```
git clone https://github.com/Davis-Garrad/DNMR.git
cd DNMR
pip install -e .
```

Once either of these versions has been installed, the program itself can be started with the command,

```
python -m DNMR
```

5 Getting Started in NICOS

This section does not cover basic setup. The purpose of this section is to get the user started collecting and saving data in a running NICOS server, with an available frappy server to connect to.

The first step in using a frappy device is connecting to it. The NICOS server may automatically connect to it, in which case the user would see some sort of "ready" status. If this is not the case, then the status will contain information on some sort of connection error:



Figure 2: A failed frappy-NICOS connection on the se_main device.

In most cases, if configured correctly, this can be fixed by reconfiguring the device's uri parameter, after which NICOS will automatically try to reconnect. This value can be found in the frappy server configuration, as well as the frappy server command output.

Now that the user has a frappy-TNMR interface configured and running in NICOS, they may want to take some data. This is simple enough, and example scripts for typical experiments are provided in {nicos}/nicos_sinq/tnmr/example_scripts. It is recommended that the user familiarises themselves with the T1 and frequency scan scripts, in particular, as they are most informative.

After one of these scripts is run, status updates will be appended to the NICOS log, as in Fig. 3 and a file will be generated containing all the data.

The datafile can be loaded into DNMR directly from the command line:

```
python -m DNMR {filename(s)}
```

or via the in-app dialogue.

Figure 3: What the start of a scan looks like in NICOS. Note the scan number, sample name, and filename. These are functionalities of NICOS. The ETA and completion time are both a function of the TNMR-frappy-NICOS system; see Sec. 6 for more detail.

In this example, a T1 scan is analysed: First, the data is loaded in and rephased. Each datapoint can be viewed, rephased, and the peak to analyse can be identified separately. For the purpose of a simple T1 scan, however, it makes the most sense to just use the auto-rephasing feature. This is illustrated in Fig. 4.

One can also, if using a particular filter which doesn't already, apply a window to the Fourier transform of the data. This will be used in integrating the data for the T1 datapoints. Regardless of whether the user needs to do this or not, the Fourier transform can be found in the "FT" tab, as shown in Fig. 5.

After the data is made ready from the previous steps, it can be viewed in a custom-made tab, built specifically for T1 scan data. Fig. 6 shows what this might look like for some particularly pleasant data, as well as a fit which was made after clicking the "Fit" button.

Now the user has, in following this example, taken, inspected, and analysed data. This concludes the "Getting Started" section.

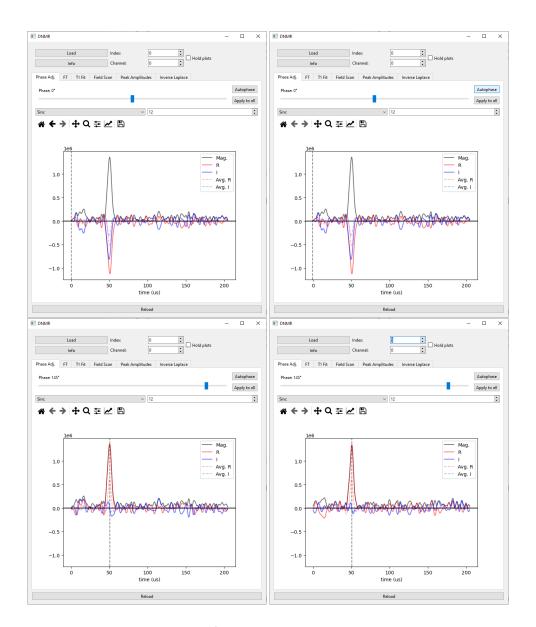


Figure 4: In a T1 analysis, the first step is rephasing the data. DNMR has an inbuilt auto-rephasing functionality, activated by clicking the button labelled "Autophase." The next step is to scroll through the different scan points (with their own "index") and verify that the data and rephasing looks reasonable.

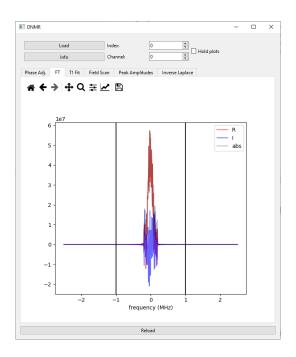


Figure 5: The Fourier transform of the data can be viewed in the "FT" tab.

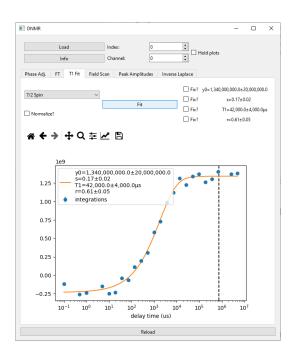


Figure 6: The "T1 Fit" tab is custom-made to perform fits on T1 data, so this is the logical next tab to visit. After pressing the "Fit" button, we can then parse the result.

6 Basic Programming Reference

In this section, commands and functions will be detailed together, but colour-coded separately. Commands (accessible to NICOS users) will be coloured blue, parameters (also accessible to NICOS users) will be coloured teal, and developer functions (accessible only behind the scenes) will be coloured grey. Section titles are the filenames in which one can find the discussed functionality, without extensions.

6.1 NICOS

User Commands

generate_pulse(pw, ph, dt, pc)

Generates a dictionary representing a pulse in a pulse sequence. Parameters are pulse width (us), pulse height (a.u., % total power for the SCOUT), delay time (us), phase cycle (str, e.g., "0 1 2 3")

```
generate_sequences(base_sequence: list,
pulse_indices: list, var_name: str, vals: list)
```

Creates a list of pulse sequences from a single pulse sequence, assigning a variable in a collection of pulses to a value in the given list. For instance, if a user wanted to scan the first and second delay times over the range 5-10us in 1us bins, they could write generate_sequences(some_base_sequence, [0,1], 'delay_time', [5,6,7,8,9,10]) to generate the appropriate list. In effect, base_sequence is copied for each entry in vals, and the value of var_name in each of the pulses indicated by pulse_indices are changed to one of the values in vals.

log_durations(s, e, N)

Generates a list of durations between s and e (inclusive), logarithmically spaced.

estimate_sequence_length(seq)

Returns the estimated time, in seconds, of a single pulse sequence acquisition.

estimate_scan_length(scan_seq)

Returns the estimated time, in seconds, of a list of pulse sequence acquisitions.

timestring(seconds)

Returns a nicely formatted string indicating a length and how far that is into the future.

print_sequence(seq)

Prints a pulse sequence nicely.

scan_sequence(dev, seq)

Given a TNMR interface dev, performs a compilation, zero-go, and saves data from the acquisition for a single pulse sequence.

scan_sequences(dev, sequence_list)

Given a TNMR interface dev, acquires data for a list of pulse sequences and bundles the data together in one file (with separate entries). This is simply the list-form of scan_sequence.

begin_tnmr_scan()

Tells the NICOS data manager that the user is manually controlling where the scan starts and ends. Useful if one needs to use scan_sequence repeatedly (instead of scan_sequences, which handles data management for scans).

finish_tnmr_scan()

Gives up manual control of the data manager.

get_tnmr_params()

Returns a dictionary of the currently loaded parameters in the TNMR interface, like acquisition time, observed frequency, and 1D scans.

6.2 Frappy

6.2.1 TNMR VisualBasic/COM Interface (tnmr_interface and NTNMR)

It is recommended to check Tecmag's TNMR documentation for detailed notes. This document does not seem to be publicly available, but can likely be sourced from the support.

6.2.2 OTFModule

Commands/Parameters accessible through SECoP

This encapsulates all the functionality that NICOS directly sees.

compile_and_run(thread=True)

Compiles and runs the currently-loaded pulse sequence and options. If thread is set to True, then this function starts a child thread. Otherwise, this function blocks.

kill()

This command sends an Abort signal to TNMR, signalling the program to halt an acquisition. This does *not* guarantee that the acquisition will end.

title

This parameter only determines what the title written into the sequence file is.

(pre,post,-)acquisition_time

See sequence_generation. Pre- and regular acquisition times in μ s, post-acquisition time in ms.

ringdown_time

See sequence_generation. In μ s

acq_phase_cycle

See sequence_generation.

num_scans

This parameter determines the total number of averaged scans for each datapoint.

obs_freq

The frequency of the receiver. In MHz.

Developer Functions

tnmr()

This function creates a new instance of the TNMR API wrapper. To be used upon every access to the TNMR software from code.

stop()

Simply provides the core functionality for kill().

__compile_sequence()

Compiles the sequence loaded in sequence_data. This involves the following:

- 1. creating the sequence table via seq_gen.get_single_pulse_block calls;
- 2. combining them all; saving this sequence where TNMR can see it, and in a format it can read;
- 3. taking a copy of all the acquisition parameters (so that if they are changed mid-acquisition, no incorrect information is written to files);
- 4. telling TNMR to read it (i.e., tnmr().load_sequence()), reloading the dashboard and parameters in the process;
- 5. and giving TNMR the correct parameters to populate the new dashboard with.

The temporary sequence file is saved in root/sequences and timestamped where root is the working directory of the frappy server command. The word "compile" is a bit of a misnomer in its usage here, but signifies that all of a pulse sequence's information is collected and prepared according to some process to ensure both that it works and that it is saved in an accessible and reproducible manner.

__zero_go()

This command simply sends a command to TNMR to begin to acquire data (Zero-and-Go). This is not meant to be called before __compile_sequence(), and the consequences of such an action are deemed undefined behaviour.

__compile_and_run()

An extremely thin wrapper for first compiling and then Zero-Going.

6.3 tnmr_interface

This module exists entirely as an API for Tecmag. Most functions are simple wrappers for the COM interface.

get_instance()

This function attempts to create or get an existing instance of a COM interface object, connected to a TNMR instance. It is important that the handle for this COM object is often refreshed (i.e., not stored in an object), as the interface can fail when new threads/processes are created and try to do the same. Treat this as a singleton pattern to avoid headaches and trouble.

execute_cmd(cmd)

Sends an arbitrary COM interface command through to TNMR. This is useful for debugging, but should not be accessible to end users, as it can destabilise things if used improperly. Think of it as a really big sledgehammer - no user should ever come close, even if *they* think they need to remove a wall.

openfile(filepath, active=True)

Opens a .TNT file into TNMR. This can provide direct access to the data and sequence used to get it. Further, it also loads some settings from the .TNT.

set_activefile()

Updates the active file and active filepath internally. (Currently unused)

ZeroGo(lock=True, interval=0.5[s], check_time=10[s])

If no acquisition is already running, signals to TNMR to Zero-and-Go. If successful in sending this signal, the function then forces a halt until some condition is met (within the function, a constant CHECK_MODE is set to either "data" or "thread". The condition for "data" is that the zeroth data point changes within check_time. The condition for "thread" is that the thread started to send the Zero-Go command terminates before check_time. Default is "thread") or check_time elapses. If check_time does elapse, this is a signal of some fault in TNMR and the function recursively tries again. Once this succeeds, if lock is enabled then every interval, TNMR is polled to see if the acquisition is complete and control is released once it is.

acquisition_running()

Returns a boolean value: whether an acquisition is currently running or not.

get_data()

Pulls all the data from TNMR and returns it as a tuple: (reals, imaginaries).

save_file(filepath=")

Saves the current setup as a .TNT file. If filepath is left as the default, then the currently active file is overwritten.

set_nmrparameter(param_name, value)

Sets a dashboard parameter. It does not matter which page the parameter is on. Eg., set_nmrparameter("0bs. Freq", "41.5MHz") has the same effect as manually changing "0bs. Freq" in TNMR to 41.5MHz.

get_nmrparameter(param_name)

Returns the value of a dashboard parameter.

is_nmrparameter(param_name)

Returns a boolean: whether the provided parameter name is found in the list of valid parameters.

get_all_nmrparameters()

Returns a dictionary of all the dashboard parameters, in the form { [page name]: { [parameter name]: [parameter value], ... }, ... }. This may result in duplicates, as parameters can be on multiple pages at once.

get_page_parameters(page)

Like get_all_nmrparameters, but for a single page.

load_sequence(filename)

Possibly destructive to live data. This is more interesting than it sounds. Sequences cannot be loaded directly as TNMR's API is slightly dodgy here. This function, in short, closes the active file (this is the destructive part), loads a template file with some default values, loads a default dashboard, loads a sequence into the template file, saves the template file into an even more temporary file, and finally re-opens that file. These acrobatics are justified in that doing anything else results in TNMR being unhappy.

load_dashboard(dashboard_fn)

Loads a dashboard from a dashboard setup file. Despite what the TNMR documentation says, this *does* seem to overwrite the values in the dashboard. Potentially useful, but not used currently.

6.3.1 sequence_generation

This file exists to hold helper functions for reading and writing pulse sequence files in Tecmag format. The structure of a pulse sequence is limited to aid in usability and simplicity. Every pulse sequence is composed of a sequence of pulses (if one cannot wrap their mind around this concept, they should be kept far from RF electronics). Each of these pulses is parameterised by 4

values:

- · Pulse width; how long the signal remains HIGH for.
- Pulse height; the power output of the signal.
- Delay time; how long to keep the signal LOW for after the pulse.
- Phase cycle; a string, of the form "0 1 2 3 3 2 1 0" which determines the phase cycling sequence. This is dependent on the hardware used.

These pulses, in Python, are stored as dictionaries with keys pulse_width, pulse_height, delay_time, and phase_cycle. These pulses (dictionaries) can be combined into a pulse sequence (list of dictionaries).

In the sequence_generation implementation the dictionaries are slightly more complicated as this is the lowest level of pulse sequence handling; they contain fields for every possibility in TNMR. There exists a helper function, combine_blocks(1, r), which should be used to combine blocks (collections of columns) in Python (TNMR). Further, all pulse sequences must be bookended by an "initial" block and a "final" block, which define phase reset, acquisition, ringdown, etc..

Functionality to create pulse sequences

```
get_single_pulse_block(name, pulse_width,
pulse_height, delay_time, phase_cycle="0")
```

Creates a single "block" dictionary for a single pulse. All times should be provided in the format "10u".

get_initial_block()

Creates a single "block" dictionary to be placed at the start of any pulse sequence.

```
get_final_block(ringdown_time, preacquire_time,
acquire_time, cooldown_time, acq_phase_cycle="0")
```

Creates a single "block" dictionary to be placed at the end of any pulse sequence. Ringdown before acquisition, a delay after ringdown (preacquire_time), acquisition time, post-acquisition delay, and the acquisition phase cycle are all configurable. All times should be provided in the format "10u".

combine_blocks(1, r)

Combines two "blocks", 1 and r, in the order: 1 first, then r.

Functionality to handle files

```
save_sequence(filename, sequence)
```

Saves a sequence to a file in Tecmag's format.

```
save_sequence_cfg(filename, sequence)
```

Saves a sequence to a file in a human-readable JSON file.

6.3.2 sequence_fileformat

This is the best documentation of the TNMR sequence file format that I could generate from inspection and trial and error. It also happens to be the file which provides some helper functions to generate proper file structure. Generally, even a developer for this software can ignore this particular interface, and limit themselves to using the sequence_generation interface.

fm(s, spacing=3)

Generates the correct string for a value in string format such that TNMR can understand it. Pretty much every value in a TNMR sequence file is formatted as such.

```
get_info_header(filename, author, col_names,
tuning_number, binary_name="PSEQ1.001.18 BIN")
```

Generates a string for the top of the sequence file, which contains information on the filename, author, columns, the number of columns (tuning_number for historical reasons), and the binary used to generate the file. While programs using this API will emphatically *not* be named "PSEQ1.001.18 BIN", this is what TNMR expects when loading a file. We always tell TNMR what it wants to hear.

get_delay_header(col_delays, tuning_number)

Generates a string for the delay section of the sequence file.

get_event_header(event_type, vals, tables, table_reg, tuning_number, col_delays)

Generates a string describing the events section of the sequence file. If tables are used anywhere in the events, they should be registered in the table registry (table_reg). This part should come after the delay section.

get_table_spec(table)

Generates the string for the table specification in the sequence file. This goes after the event section.

generate_default_sequence(col_names, col_delays)

Generates a dictionary containing all the necessary information to provide a solid base to make small adjustments to. Default values can be found in the sequence_fileformat.py file, under event_defaults. The generated dictionary should be passed to create_sequence_file after adjustments.

create_sequence_file(filename, data, author="NA")

Takes a dictionary with all possible information that Tecmag could possibly require, and generates a .TPS Tecmag pulse sequence file from it. The helper function generate_default_sequence can be useful here.

7 Drawbacks, Known Issues, and Other Notes

- Only Linux is supported for the NICOS server. This is due to the use of os.fork, technically a part of Python's standard library but very much not cross-platform. Since no TNMR program exists for Linux, this means that two computers are necessary for this setup. Fortunately, one of them can also act as "master" for the rest of the setup, and the TNMR PC can be somewhat isolated.
- If there is some problem in TNMR that requires intervention, the acquisition commands will recursively retry, possibly leading to a stack overflow and therefore a crash of the frappy server. This, in the author's experience, has never happened in reality but it is quite possible in theory.