Atomize: open source modular software for working with scientific devices

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Abstract

Remote control of spectrometers is usually carried out using home-written programs, which are restricted to doing a certain experiment with a specific set of devices. The programs like fsc2 [1] or Atomize [2] are much more flexible, since they are based on a modular approach for communication with device and scripting language for data measuring.

The user interface (UI) of Atomize was created with PyQt. One- and two-dimensional graphs are plotted using the highly productive library pyqtgraph. The software has modules for controlling various parts of the spectrometer, e.g., temperature controllers, digitizers, etc., with the hardware details hidden. The programming interface calls high-level functions with self-explanatory names, e.g., *digitizer_get_curve()*.

The modular approach used makes it easy to incrementally update the spectrometer with newer components or more advanced devices without any changes to the main program.

Supported devices

At the moment, Atomize supports over 30 different devices, including 4 series of devices:

1. Lock-In Amplifiers
SR-810; SR-830; SR-850; SR-860; SR-865a

2. Oscilloscopes
Tektronix 4000 Series;
Keysight Infinii Vision 2000, 3000, 4000 X-Series

3. Digitizers
Spectrum M4I 4450 X8

4. Temperature Controllers
Lakeshore 325; 331; 332; 335; 336; 340;
Oxford Instr. ITC-503; Termodat 11M6; 13KX3;
SR-PTC10; Scientific Instr. SCM10

5. Magnetic Field Controllers
Bruker BH15; ER032M; ER031M

6. Microwave Bridge Controllers
Mikran X-band MW Bridge

7. Arbitrary Wave Generators
Spectrum M4I 6631 X8

8. Pulse Programmers
Pulse Blaster ESR 500 Pro

9. Power Supplies
Rigol DP800 Series; SR-DC205; SR-PS300

10. Frequency Counters
Agilent 53181A; 53131A/132A;
Keysight 53230A/220A

11. Gaussmeters
Lakeshore 455 DSP

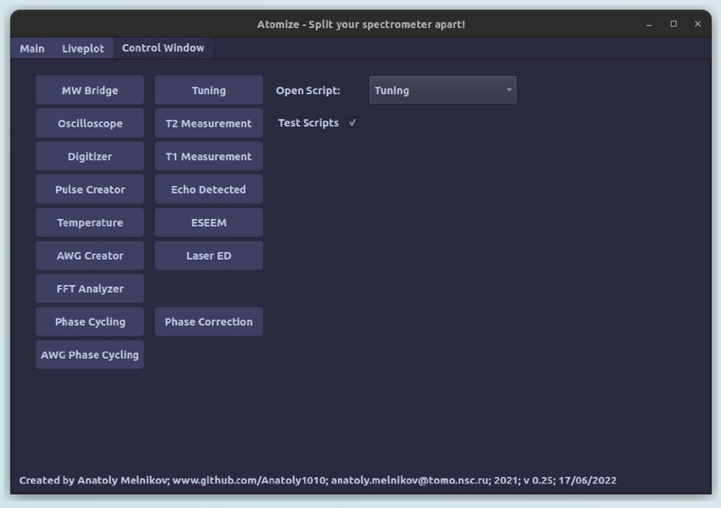
12. Delay Generators
SR-DG535

13. Others
RODOS-10N Solid-State Relay;
Owen-MK110-220.4DN.4R Discrete IO Module;
Cryomagnetics LM-510 Liquid Cryogen Monitor;
Cryomech CPA2896, CPA1110 Digital Panels;
CPWplus 150 Balance

Applications

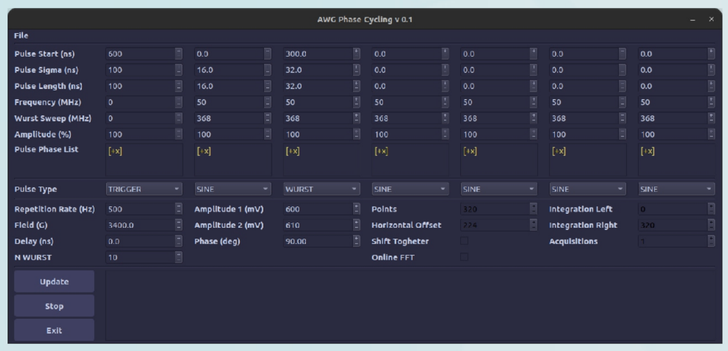
I. Pulsed EPR with AWG unit

Full control of a home-made pulsed EPR spectrometer, including rectangular and AWG pulse tables, presets for typical measurements, UI for controlling diferent devices, and data processing tools.



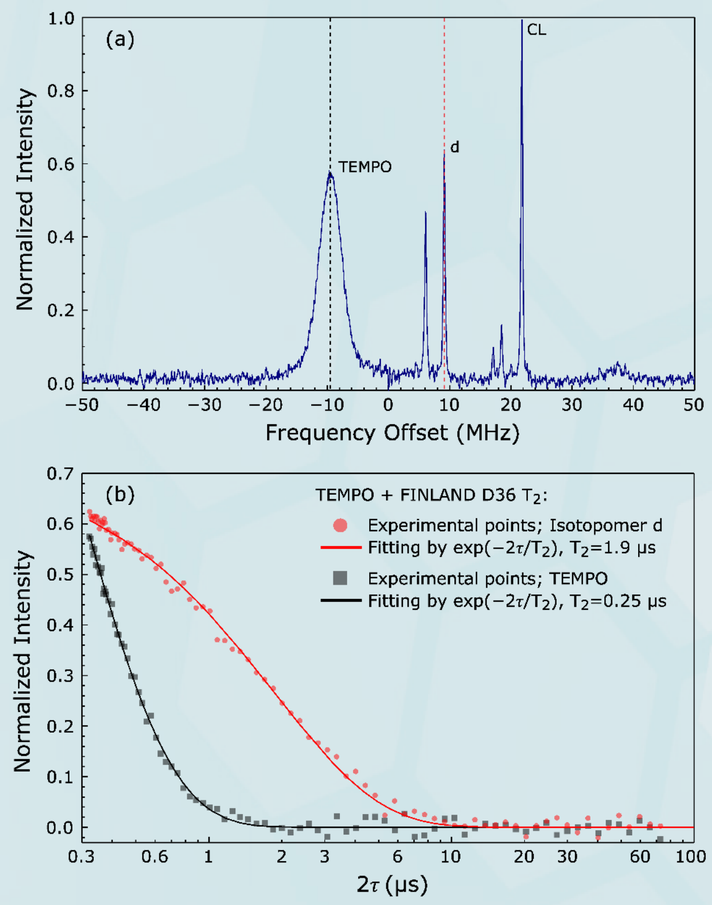
Online phase cycling and FFT

Pulse tables include a possibility of on-the-fly phase cycling. The use of the C or C++ backend of the ADC, DAC, and pulse programmer provides fast updates of data plots or their FFTs with a refresh of 100 Hz if it is allowed by experimental data accumulation rate.



Non-uniform sampling

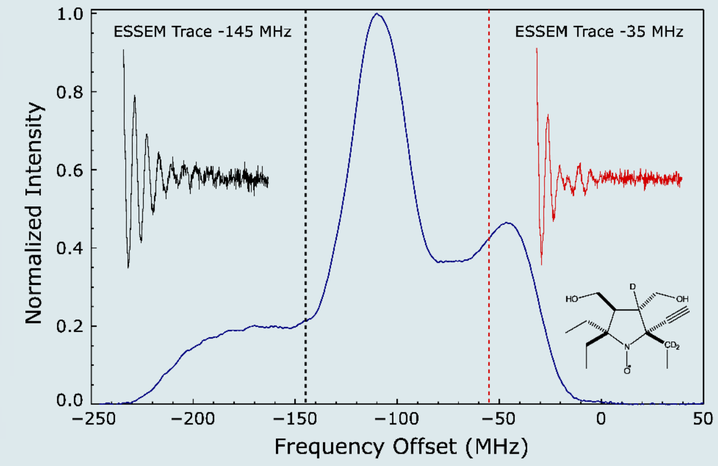
All pulse sequences can be setup with non-uniform sampling that provides better sensitivity for DEER, HYSCORE, T_1, and T_2 experiments.



Two pulse echo measurements of 30 μM TEMPO and 10 μM Finland trityl D36. (a) Phase corrected FT spectrum at 170 ns; (b) echo decay for the high field TEMPO line and for the high field line of the trityl isotopomer 'd'.

Full nitroxide excitation

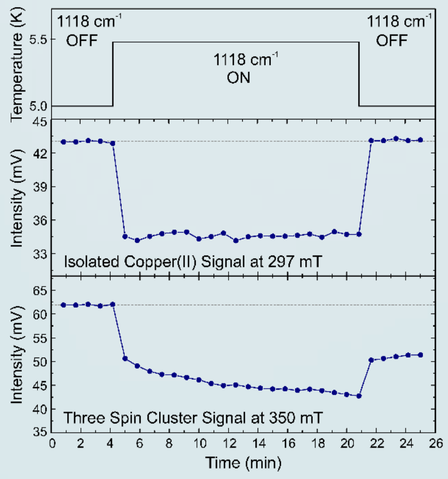
The AWG unit allows using adiabatic pulses such as WURST to excite the entire radical spectrum with a width of about 300 MHz.



Phase corrected FT spectrum of nitroxide obtained using WURST pulses and its ESEEM traces at -145 and -35 MHz offsets.

II. Continuous wave EPR

Full control of the CW and TR EPR spectrometer, located at Novosibirsk Free Electron Laser facility.

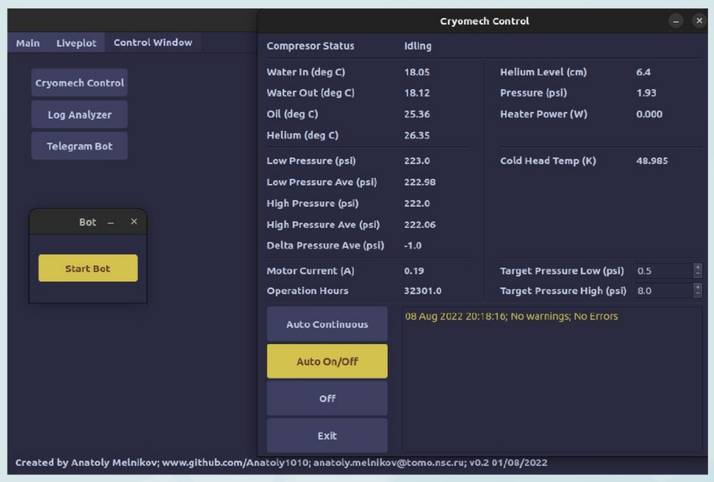


Automatic adjustment of the NovoFEL repetition rate to ensure that the sample is irradiated with constant power.

See also Poster #054.

III. Cryomech liquid helium plant

UI for controlling Cryomech LHeP22, allowing switching between different modes of operation of the plant and remote control via Telegram bot.



Conclusions

Herein, we report the current status of Atomize, an open source modular software for working with scientific devices. There are more than 200 device specific, general, and plotting functions available for over 30 different devices, including 4 series of devices. Atomize has been tested on Ubuntu 18.04, 20.04, and 22.04 and is currently used for controlling several spectrometers. The source code is available at https://github.com/Anatoly1010/Atomize

Poster #053

Star us at github!

[1] http://fsc2.org
[2] https://github.com/Anatoly1010/Atomize

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