SpecMan4EPR

A versatile control software for pulse EPR

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Introduction

The rapid development of modern state-of-the-art pulse EPR spectroscopy constantly creates new instrumental challenges. Many research groups develop their own instruments with unique features. Construction of a spectrometer requires a broad expertise, both in microwave electronics and acquisition hardware. However, what really makes the assembly of equipment into a robust and useful tool is its front-end, the control software. Often, home-built software has a lab lifetime of the student(s) who wrote it and usually does not benefit from the advantages of testing in different environments or the support of dedicated staff who understand both the hardware and software of an EPR instrument.

SpecMan4EPR is a comprehensive and inexpensive solution to this problem.

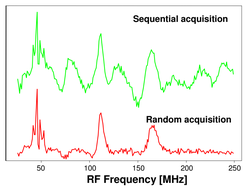
SpecMan4EPR was introduced as a collaborative project between the groups of Prof. Daniella Goldfarb, Weizmann Institute of Science and Prof. Arthur Schweiger, Swiss Federal Institute of Technology (ETH), Switzerland.[1] The initial design of the software was carried out by BE, Dr. Stefan Stoll (currently Department of Chemistry, University of California, Davis, CA) and Dr. Igor Gromov (currently Bruker Biospin, Germany). Imaging and real time communication features were developed in collaboration with the Center for EPR Imaging In Vivo Physiology, University of Chicago, NIH grants number P41 EB002034, R01 CA98575.

Presently SpecMan4EPR is a commercial product marketed by Scientific Software Services.[2] Full support and services are available.

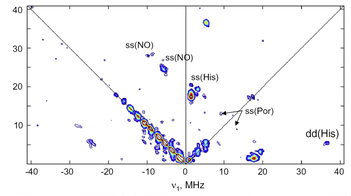
1. Epel *et al.*, Concepts in Magn Reson B 2005, 26B, 36.
2. http://www.scientific-software.com/; http://www.specman4epr.com/

Applications

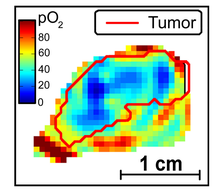
Currently SpecMan4EPR is employed for a wide spectrum of applications in different laboratories. Although pulse EPR is the primary use of the program, many investigators take advantage of the program's flexibility to control continuous wave, DNP and other EPR instruments. Recently SpecMan4EPR was upgraded to include imaging capabilities.



^{55}Mn ENDOR of [Mn(II)Mn(III)(μ-OH)(μ-piv)$_2$(Me$_3$tacn)$_2$](ClO$_4$)$_2$. Max Plank Institute for Bioinorganic Chemistry, Germany, 2005.



**A W - band HYSCORE spectrum of myglobin-NO system.
Goldfarb, D. *et al.* JMR 2008, 194, 8-15.**

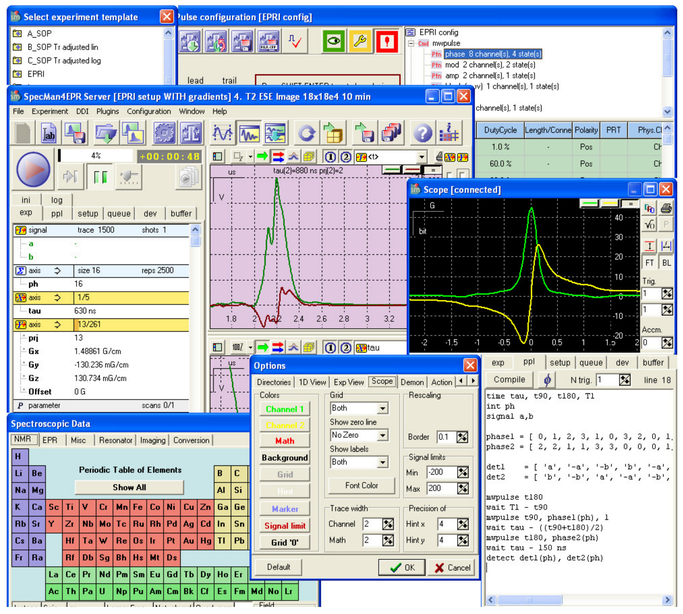


Electron spin echo oxygen image of a mouse leg bearing a tumor. OX063 spin probe. Courtesy of Prof. Halpern H.J., University of Chicago, 2010.

Features

Device drivers

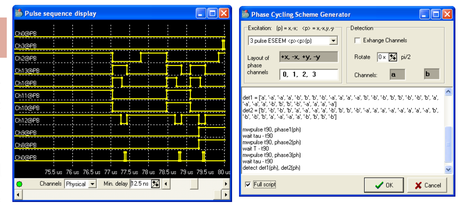
The most important advantage of SpecMan4EPR is its ability to utilize third party devices to control an instrument. Currently more than 25 devices frequently used in EPR are supported. New devices are continually added. SpecMan4EPR is compatible with National Instruments™ traditional DAQ and DAQmx hardware and has generic support for AT&T style command-based protocols over GPIB, USB, COM and TCP-IP. All devices are seamlessly integrated into the program and do not require any knowledge of underlying protocols. SpecMan4EPR core algorithms handle synchronicity and other aspects of device control without any input from the user. Wizards simplify addition and configuration of hardware.



Experiment

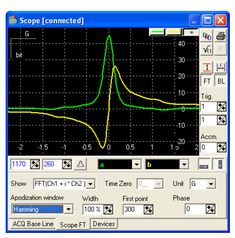
SpecMan4EPR supports five dimensional experiments. Two of these dimensions represent transient signal and multiple triggers per sequence. The parameters of the other dimensions can have linear, logarithmic or look-up table definition. Any device property (for example frequency or power of an RF source) can be a parameter of the experiment. The experiment can be executed in sequential or random order.

PPL



Pulse experiments are codified using pulse programming language (PPL). The actions of all PPL commands are defined by the pulse configuration wizard. Each command can create multiple pulses enabling the use of very sophisticated patterns. For user convenience, calculated sequences can be visualized in real time. Phase cycling schemes and sequence generators are available for common sequences.

Digital scope

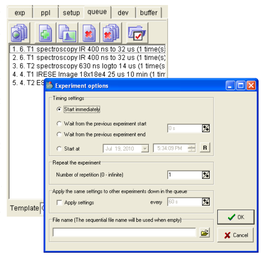


Pulse spectrometers commonly use transient digitizers for signal detection. The same transient signal can be employed for tuning the spectrometer and optimizing an experiment.

SpecMan4EPR has a Digital scope facility with multiple options frequently found in stand alone oscilloscopes. The Scope can display the raw input signal, average it, take the absolute value of the quadrature signal, or perform complex Fourier transformation of the signal. The range of integration for boxcar-like detection is controlled from the Scope as well. For visualization of weak signals riding on a strong baseline the Scope can store a baseline trace recorded in the absence of signal (for example at magnetic field far off-resonance) and dynamically subtract it from the signal.

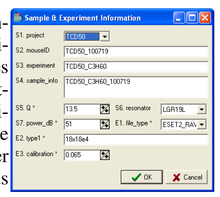
For user convenience any device parameter or action control can be added to the Scope panel.

Queue of experiments



Frequently the user wants to execute multiple experiments in continuous fashion. SpecMan4EPR allows the user to submit any sequence of experiments to the queue. The execution time and number of repetitions can be specified for each experiment in the queue. Single experiments or groups of experiments can be repeated indefinitely as desired.

Information organizer



This feature allows the user to create information fields stored into the experiment file. The user may choose the names and types of the fields. Experiment-specific fields are associated with experiment templates. Sample-specific fields are preserved from one experiment to another until changed. The user may change fields while experiments are running.

http://www.specman4epr.com

SpecMan4EPR continuously absorbs new developments in the field of EPR instrumentation. The information about recent additions to the program and manual are available online. A fully functional demo version of the program can be downloaded from our site.

We welcome any suggestion for improvement of the software - feel free to contact the development team.

Client-Server Edition

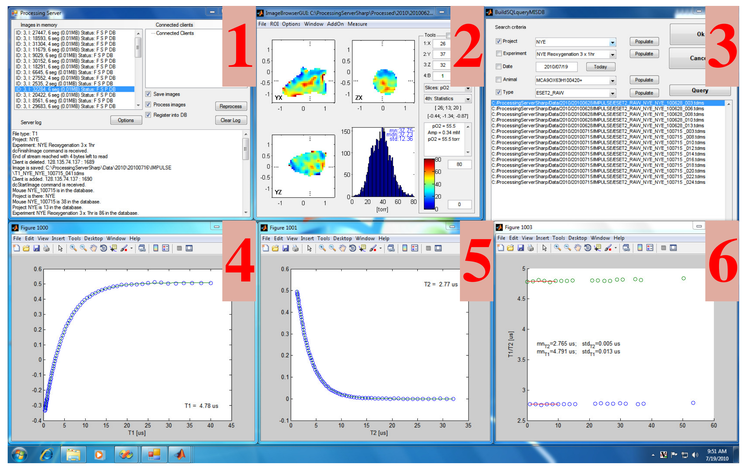
This is the basic edition of the program. It can be used for pulse, CW, DNP or any other instruments. SpecMan4EPR is built using client-server technology. The server part of the program that controls hardware can be located at your lab miles away, while the user interface will be right on the desktop of your computer. Custom TCP-IP protocol is used for communication.

System requirements: 32-bit or compatible MS Windows OS (Windows 7 and Vista compatible), drivers for third party devices.

Imaging Edition

Rapid development of pulse EPR imaging applications inspired the modification of the program core. The gigabyte-size multidimensional arrays of data obtained during imaging require special care in management of computer memory and network bandwidth. SpecMan4EPR currently handles experiments with up to 600 MB of data and we are working to increase this limit.

Another important feature of the Imaging Edition is the ability to transfer data during the experiment to other applications. This is especially important for EPR imaging of live animals. An investigator making EPR images of live animals benefits from real time data on concentration of spin probe, oxygenation and other parameters as the animal is being imaged. In order to provide this feedback raw imaging data has to be processed using sophisticated algorithms, which require considerable computing power. These computational demands can overburden the acquisition station and therefore should be performed on a separate computer. We have implemented TCP-IP data transfer using the TDMS protocol developed by National Instruments™. On the screenshot below, the Processing Server application receives data from various experiments from a SpecMan4EPR based console and processes them using experiment specific algorithms.



1 - User interface of the Processing Server application developed at the Center for EPR Imaging In Vivo Physiology, University of Chicago. Data are collected from 250 MHz pulse EPR imager controlled by SpecMan4EPR. Currently three Processing Server modules are implemented: data storage, MATLAB™ data processing, and an SQL database interface.

2 - MATLAB™ user interface of the image processing toolbox developed at the University of Chicago featuring real time reconstruction of an electron spin echo image of the tumor bearing leg of a mouse.

3 - User interface of the query builder for the animal imaging SQL database.

4, 5, 6 - MATLAB™ generated figures displaying results of real time processing of inversion recovery and electron spin echo decay experiments. Figure 6 shows time dependence of relaxation times for sequential measurements on the same sample. Data to MATLAB™ are supplied by Processing Server.