


## Package name: EPRSIM C – technical information

### Program name: EPRSIM WIZ

Icon: 

OS environment: MS Windows (32 bit)

Windows application – user interface

Version & Release: 6.2.2

Purpose:

- handling EPR data – opening spectral files, creating multiple experiment MTP files – collecting or combining EPR experiments, saving files (corrected baseline, normalized), integration, difference,
- local DSO spectra optimization (fine tuning),
- connection to EPRSIM Master for Cluster mode

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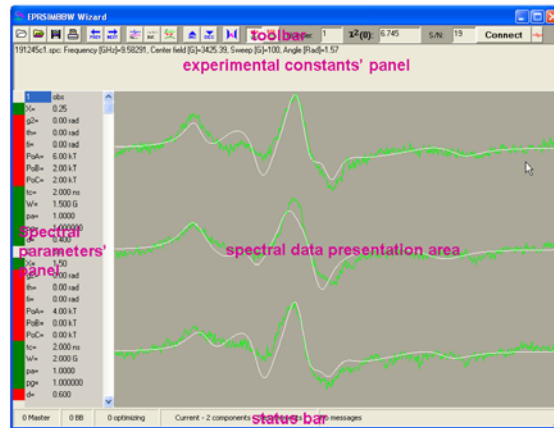
## 1 EPRSIM WIZ user interface

EPRSIM WIZ program of the EPRSIM C package is designed to handle experimental and simulation data from multiple series of EPR experiments and to combine this data into MTP files or send it directly to EPRSIM C cluster (if setup).

EPRSIM WIZ is based on the graphical interface that changes automatically regarding the type of experiment and simulation model applied.

The graphical interface is divided into 5 areas as presented on the picture below:

- *spectral data presentation area*
- *spectral parameters' panel*
- *experimental constants' panel*
- *toolbar*
- *status bar*



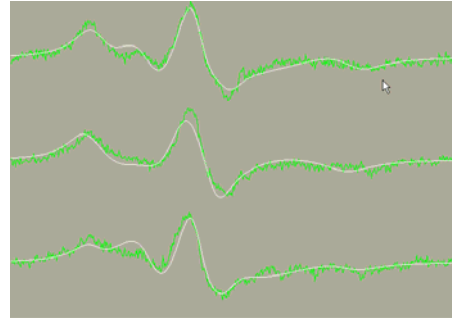
The structure and function of the particular areas are defined in the subsections below.

## 1.1 Spectral data presentation

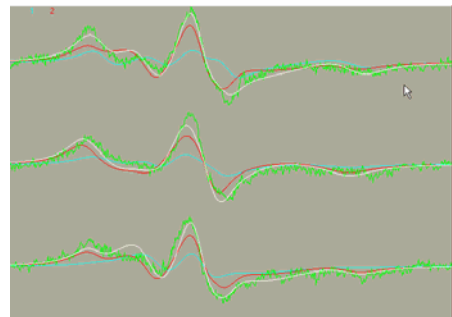
The main area of the EPRSIM WIZ window is devoted to spectra presentation.

Green spectra are experimental ones.  
White spectra are simulated ones.

If multifrequency or multiangle experiment is under investigation, connected experiments are presented at the same time at different vertical position.



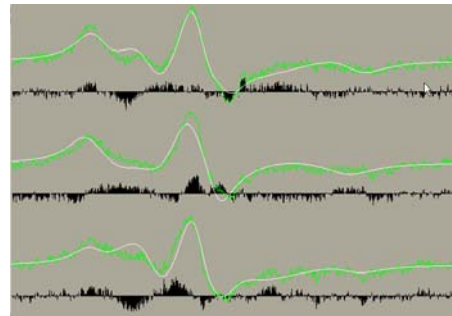
If desired (see [Toolbar](#)), the spectral components are presented in colors and indicated by the color-numbered index in the top-left corner of the *presentation panel*.



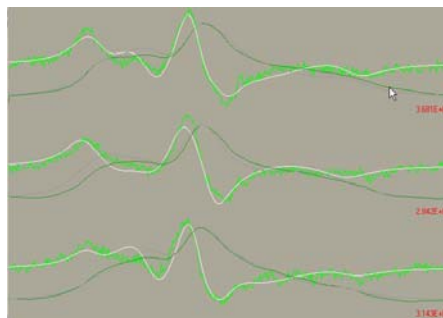
If multifrequency or multiangle experiment is under investigation, all the components are presented for all the experimental spectra on the panel.

If desired (see [Toolbar](#)), the difference between experimental and simulated spectra are presented in black below the spectra.

If multifrequency or multiangle experiment is under investigation, all the difference spectra are presented for all the experimental spectra on the panel.



If desired (see [Toolbar](#)), the first integrals of the experimental and simulated spectra are presented in dark green and gray, respectively above the same reference line as is used for presenting difference.



If multifrequency or multiangle experiment is under investigation, first integrals are shown for all the experiments.

In addition, double integrals (spectral intensities) are shown on the right side of the spectra, just below the reference line. The baseline correction is already taken into account.

## 1.2 Spectral parameter panel

Spectral parameters that are used to determine spectral components in the spectral simulation are presented on the *spectral parameter panel*, left from spectral presentation area.

Spectral parameters are grouped for spectral components, group (spectral component or domain) is indicated by its number and type in the first line of the group.

For model types and explanation of spectral parameters that are used for particular model see [EPRSIM Library](#).

Spectral parameters can be modified by simple write the number in the appropriate cells without the units which are added automatically. The spectral parameters' values can also be change by the up/down buttons on the toolbar (see [Toolbar section](#)).

On the left side of the panel, the parameters' switches are shown. The red squares represent locked parameters (cannot be optimized) whereas the green ones represent the unlocked parameters (those that will be optimized. Note that the weight of the last component is always locked (red). The switch can be changed by double-clicking on the colored squares.

Use the scrollbar at right of the panel to scroll up/down to reach/see all the parameters and switches.

1	obs
X=	0.25
g2=	0.00 rad
th=	0.00 rad
fi=	0.00 rad
PoA=	6.00 kT
PoB=	2.00 kT
PoC=	2.00 kT
tc=	2.000 ns
W=	1.500 G
pa=	1.0000
pg=	1.000000
d=	0.400
2	obs
X=	1.50
g2=	0.00 rad
th=	0.00 rad
fi=	0.00 rad
PoA=	4.00 kT
PoB=	0.00 kT
PoC=	0.00 kT
tc=	2.000 ns
W=	2.000 G
pa=	1.0000
pg=	1.000000
d=	0.600

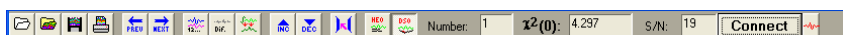
## 1.3 Experimental constants' panel

The following data about the experiments are shown in the *experimental constants* panel: spectral filenames, frequency, center field, sweep and angle. If needed one can modify the values by double-clicking the panel to reach appropriate dialog box (see [Handling EPR data](#) section and [Creating MTP data sets](#) subsection). Double-click has no effect until at least one spectral file is loaded, i.e. new MTP series is constructed first.















In the same dialog box, one can modify number of components and their types. Moreover, one can also add new spectral datasets or change existing ones.




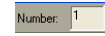
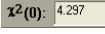




When modifying already existing spectral components by changing its type, EPRSIM WIZ uses spectral parameters from old type for the new type if possible.

## 1.4 Toolbar

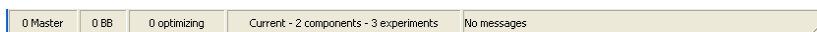


Toolbar includes all the important buttons and information text-holders. Their function is presented on the table below:

- |   |   |
|---|---|
|  | ... <a href="#">Creating the new MTP</a> by collecting experimental data – spectra, frequencies, field, sweeps, angles – and defining the number and types of spectral components   |
|  | ... <a href="#">Opening existing MTP file</a> which includes all the information about EPR experiment and simulation  |
|  | ... <a href="#">Saving MTP file</a> (not possible until at least one spectral file is loaded)<br> - hold SHIFT to save the current experiment only (instead of multiple series)                                      |
|  | ... <a href="#">Printing</a> experiments and simulations (not possible until at least one spectral file is loaded);<br>A dialog box opens to determine whether to print also system constants, spectral components and to decide whether to print current experiment only or the whole multiple series. |
|  | ... Move to previous experiment.  |
|  | ... Move to next experiment.  |
|  | ... Show/Hide spectral components (toggle mode).  |
|  | ... Show/Hide difference between experimental and simulated spectrum (toggle mode).   |
|  | ... Show/Hide first integral of the experimental and simulated spectrum (toggle mode).  |
|  | ... Decrease selected parameter<br> - hold SHIFT and click to decrease for 10 steps; hold CTRL and click to reach lower limit.   |
|  | ... Increase selected parameter<br> - hold SHIFT and click to increase for 10 steps; hold CTRL and   |

- click to reach upper limit.
-  ... Recenter simulated spectrum (rarely needed as the automatic routine takes care of this).
  -  ... Choose HEO as an optimization routine for this MTP multiple series. See [EPRSIM Library](#) for implementation notes.
  -  ... Choose DSO as an optimization routine for this MTP multiple series. See [EPRSIM Library](#) for implementation notes.
  -  ... Current experiment number.
  -  ... Goodness (quality) of fit  $\chi^2$  of the current experiment – if this is multifrequency or multiangle experiment, this is sum of all  $\chi^2$ .  
 - double-click on the white text-holder to toggle between standard  $\chi^2$  and first-order island-weighted  $\chi^2$ . See [EPRSIM Library](#) for definitions.
  -  ... Signal-to-noise ratio of the current experimental spectrum.
  -  ... For starting optimizations (in non CLUSTER conditions, the button caption is “Local optimization”):
    - simple click for connecting to EPRSIM master in [Cluster mode](#) and send all the problem simultaneously to clusters’ BBW working threads or
    - hold SHIFT and click for [local optimization of current problem](#) only
 NOTE that only DSO can be applied for local optimization (DSO should be chosen as an optimization routine).
  -  ... Save only spectral data (experimental and simulated) into single ASCII file.

## 1.5 Status bar



*Status bar* reports about the activity of EPRSIM WIZ.

The first two left cells are meant to report the current available [cluster](#) structure by notifying us about EPRSIM Master connected to this EPRSIM WIZ and about the number of [EPRSIM BBW](#) mains connected to Master.

Next cell reports about how many problems are being optimized either in a cluster or [locally](#).


The first larger cell includes information about current experiment – how many components and how many experiments it involves.

The last cell reports about the current activity of the EPRSIM WIZ. For example: current [local optimization](#), opening or saving MTP, error calculation, etc.

## 2 EPRSIM WIZ – handling EPR data

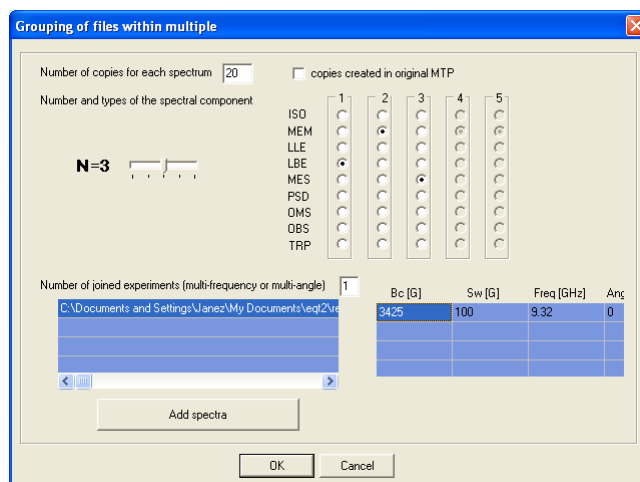
In this section one can find details how to apply EPRSIM WIZ for different tasks.

## 2.1 Creating MTP data sets

To create new MTP from spectral datasets, one has to click the  icon (1<sup>st</sup> button in [Toolbar](#)).

Additional window “Grouping of files within multiple” appears to define the following details:


- Number and types of spectral components
- Number and data about each experimental dataset:
  - spectral datasets file (multiple files can be selected for multiple series)
  - frequencies
  - center field
  - sweeps
  - angles
- Number of copies – optimization runs for each experimental problem




Drag the trackbar to change the number of spectral components. Choose in radio-groups for component type, type-in the cells for defining numbers, add files by clicking the “Add” button or double click the empty cell for filenames.


Check the “copies created in original MTP” to write down all the copies in the MTP as they would be independent problems. Do not check this checkbox to write down number of copies as a parameter send to BBW.

## 2.2 Opening existing MTP files


To open existing MTP file with all spectral files involved (filenames should be correct in order to finish this task), click  icon (2<sup>nd</sup> button of the [Toolbar](#)).

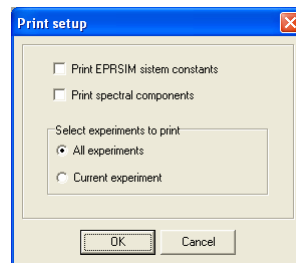
## 2.3 Saving MTP files

To save all the experimental problems defined in the whole multiple series together with all the simulated spectra, spectral components and additional experimental spectra with corrected baseline click  icon (3<sup>rd</sup> button on the [Toolbar](#)).





To save only the current experimental problem (that you currently see on the *presentation panel*) hold SHIFT and click  icon (3<sup>rd</sup> button on the [Toolbar](#)).




## 2.4 Printing



To print EPR spectral data together with different information click  icon (4<sup>th</sup> button on the [Toolbar](#)). Dialog box “Print Setup” will open to determine whether to print also system constants, spectral components and to decide whether to print current experiment only or the whole multiple series.




## 2.5 Manipulation within MTP data sets



One can change the current experiment (within the series of multiple experiments) by using two navigation buttons  and  (5<sup>th</sup> and 6<sup>th</sup> buttons on the [Toolbar](#)). You can jump from first problem to the last by pressing “previous” button  and from the last to the first by clicking “next” button .

For current problem one can show/hide spectral components by clicking , show/hide difference between experimental and simulated spectrum by clicking , and show/hide first integral of the experimental and simulated spectrum by clicking .

To change parameters without typing their values into the cells of [spectral parameter panel](#) one can select desired parameter and click  or  for increasing or decreasing selected parameters in steps defined in [MTP](#) (“Grids:” section or default). By holding SHIFT and clicking one of the two buttons, one can move for 10 steps. By holding CTRL and clicking one of the two buttons, one can move to upper or lower limit (for example to see the responsiveness of the model).

By clicking on  one can force program to recenter simulated spectrum (rarely needed as the automatic routine takes care of this).

## 2.6 Optimization control

To define which optimization routine will be used, click either  or  for HEO or DSO respectively. See [EPRSIM Library](#) for implementation notes on both optimization routines.

Note, that by choosing HEO one cannot run local optimization. On the other hand DSO can only be used for fine tuning of the solutions as it does not involve global search.



## **2.7 Defining goodness of fit (type of $\chi^2$ )**

The EPR spectrum can involve broad as well as sharp lines. Different measures of goodness of fit can therefore perform differently as a guide in optimization routine.

EPRSIM C package provide you two different functions – standard  $\chi^2$  and first-order island-weighted  $\chi^2$ . See [EPRSIM Library](#) for implementation notes on both measures. The standard  $\chi^2$  can be more efficient in optimizations of spectral parameters that should describe similar lineshapes (linewidth and lineheights). However, first-order island-weighted  $\chi^2$  performs better in spectra that are mixture of sharper and broader lines.

## **3 EPRSIM WIZ – user interface to EPR-based characterization**

Basic idea of EPRSIM WIZ is to prepare multiple experimental series for EPR-based characterization / automatic optimization via multiple runs of HEO. The later can provide solutions used to construct GHOST patterns – solution distributions – one of the direction to characterize complex systems.


As already single HEO optimization cannot be performed in time scale of seconds (like DSO) but needs 5-30 minutes depending on the model and speed of the computer, one can guess that multiple optimizations needed to construct distribution of solutions, take much more time. Therefore, data in MTP files should be primarily sent to many EPRSIM BBW programs running in parallel on different processors.

### **3.1 Sending optimization task to cluster**

The load balancing (of multiple HEO runs) can be automatic (cluster mode) or manual (resident or single run mode).

To establish local cluster one need to run single instance of EPRSIM master, as much as possible of EPRSIM BBW instances (one per motherboard recommended) and temporary EPRSIM WIZ instances that send job to cluster. Note that BBW can run parallel optimization in different working threads (number of threads is recommended to be the same as number of processors on the board).

See EPRSIM Master technical documentation for the information about establishing cluster.



To connect to EPRSIM Master one has to construct new or open an existing MTP file containing all the information about the experiments and click  button to establish connection to cluster. To start optimization one has than send the job to master by clicking the same button. EPRSIM master will balance the load through existing working EPRSIM BBWs.



After the whole job is finished, the EPRSIM master will collect the solutions and return to your instance of EPRSIM WIZ.

### **3.2 Local optimization**

Sometimes no global search is needed as in the case of fine tuning of the spectral parameters which can be known from some similar experiments on very similar or the same system under very similar conditions. In such a case one can send current problem for optimization locally.

For local optimization of current problem only hold SHIFT and click  button. Note, that only DSO can be applied for local optimization (DSO should be chosen as an optimization routine by clicking  button).