

## EPR Simulator 3.3

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### Description

*EPR simulator* is a standalone application demonstrating the basics of EPR spectroscopy. It is written in *MATLAB*, using some functions of the [EasySpin](#) package.

### Requirements

- Windows 10+ / Mac OS / Linux
- *MATLAB Runtime* libraries, version R2023b (23.2)

### Installation

*EPR Simulator* doesn't require an installation on your system, the portable version is provided. It is required though an installation of the *MATLAB Runtime* libraries, which are available online:

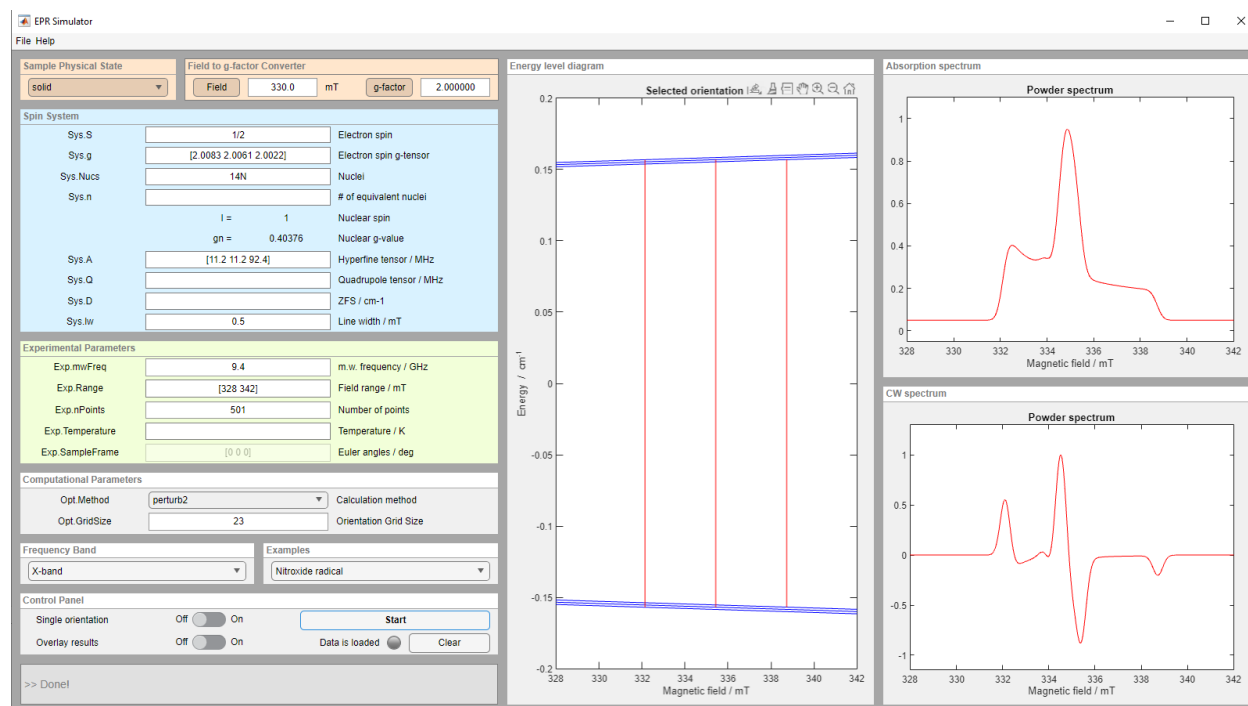
<https://www.mathworks.com/products/compiler/matlab-runtime.html>

Please make sure you install the right version of the *MATLAB Runtime* libraries.

## How to use the EPR Simulator package

### Interface

There are several panels in the main window of the *EPR Simulator*.



**SAMPLE PHYSICAL STATE PANEL** defines which of the 'easyspin' spectral simulation function will be employed, based on the sample physical state. Currently two functions are supported:

- garlic – liquid state samples (isotropic)
- pepper – solid state samples

**FIELD TO G-FACTOR CONVERTER PANEL** is a basic converter to estimate the effective g-value for a corresponding magnetic field position and the given microwave frequency

**SPIN SYSTEM PARAMETERS PANEL** is used to set up the spin system parameters, such as spin, g-value, list of nuclei, etc. The labels used for different spin system elements are the same as those used in the *EasySpin* package.

**EXPERIMENTAL PARAMETERS PANEL** defines the experimental parameters like microwave frequency, magnetic field range, the spectral resolution, and the sample orientation relative to the laboratory frame (see full description here: [easyspin docu on frames](#)).

**COMPUTATIONAL PARAMETERS PANEL** defines the calculation method and the orientational grid size.

**FREQUENCY BAND PANEL** allows you to select the resonance frequency band. Note that it changes the experimental range = [Hmin Hmax] to a full magnet range that is typically accessible in the lab.

**EXAMPLES PANEL** provides a selection of examples. Each option loads a full set of preassigned parameters.

With the **CONTROL PANEL** you can run EPR spectra simulation.

## Spin system parameters

EPR Simulator	EasySpin	Example	Description
<b>Sys.S</b>	Sys.S	0.5	Electronic spin quantum number
<b>Sys.g</b>	Sys.g	[2.01 2.004 2.001]	g-tensor
<b>Sys.Nucs</b>	Sys.Nucs	'14N'	Type of nucleus
<b>Sys.n</b>	Sys.nNucs	2	Number of equivalent nuclei
<b>I</b>	-	1	Nuclear spin quantum number
<b>g<sub>n</sub></b>	-	0.40376	Nuclear g-value
<b>Sys.A</b>	Sys.A	[10 10 90]	Hyperfine tensor / MHz
<b>Sys.Q</b>	Sys.Q	[Q η]	Quadrupole tensor (I>1/2) / MHz
<b>Sys.D</b>	Sys.D	[D E]	Zero-field splitting (S>1/2) / cm <sup>-1</sup>
<b>Sys.lw</b>	Sys.lw	0.5	EPR linewidth / mT

## Experimental parameters

EPR Simulator	EasySpin	Example	Description
<b>Exp.mwFreq</b>	Exp.mwFreq	9.4	Resonance frequency / GHz
<b>Exp.Range</b>	Exp.Range	[320 340]	Field range / mT
<b>Exp.nPoints</b>	Exp.nPoints	501	Number of points in spectrum
<b>Exp.Temperature</b>	Exp.Temperature	298	Temperature / K
<b>Exp.SampleFrame</b>	Exp.Sample	[0 90 0]	Orientation selection* / deg



\* EasySpin provides the full flexibility on defining coordinate frames, starting from a 'lab frame' to a 'tensor frame'. For a simplicity, only the 'sample frame' is taken into account meaning we can select the sample orientation within the lab frame, and it is assumed that the 'molecule frame' is collinear with the 'sample frame'. For more details read EasySpin documentation.

Number of points (**nPoints**) has to be sufficient, that the spectral resolution, defined as

$$dH = \frac{H_{max} - H_{min}}{nPoints - 1}$$

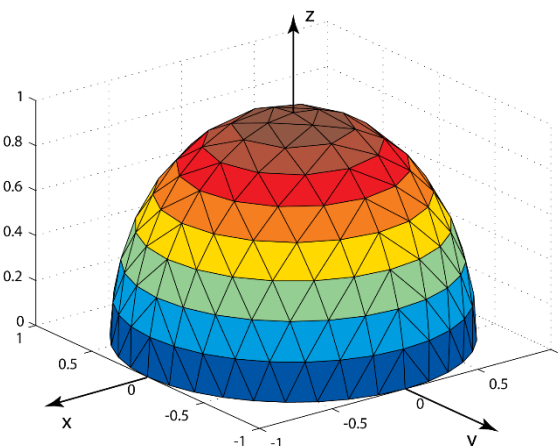
is smaller than the EPR linewidth.

## Computational parameters

EPR Simulator	EasySpin	Example	Description
Opt.Method	Opt.Method	9.4	Resonance frequency / GHz
Opt.GridSize	Opt.GridSize	31	Angle grid size

The grid size parameter (**GridSize**) defines the grid over the unit sphere used to sample the orientation of the molecule in the magnetic field (laboratory frame). The input value defines a number of points on the segment of the sphere, where  $[\varphi \ \theta]$  take values from 0 to  $\pi/2$ .

For example, for the *GridSize* = 10 (shown in the figure on the right) the  $\theta$  step is  $90 / (\text{GridSize} - 1)$ , which equals 10 degrees. The corresponding  $\varphi$  angles are calculated in the same manner. The powder spectrum is an average over single orientation spectra of each knot on the grid.



## Examples

There are several prebuilt examples showcasing EPR spectroscopy basics and some typical applications:

<b>‘Free electron’</b>	spin system of a free electron: $S=1/2$ , isotropic g-tensor;
<b>‘1 Proton’</b>	spin system of one proton: $S=1/2$ ; 1 nucleus ( $^1\text{H}$ ), isotropic g- and hyperfine tensors;
<b>‘2 Protons’</b>	spin system of two proton: $S=1/2$ ; 2 nuclei ( $^1\text{H}$ ), isotropic g- and hyperfine tensors;
<b>‘Nitroxide radical’</b>	spin system of a nitroxide radical: $S=1/2$ ; 1 nucleus ( $^{14}\text{N}$ ), anisotropic g and hyperfine tensors;
<b>‘Methyl radical’</b>	spin system of a methyl radical: $S=1/2$ ; 4 nuclei ( $3 \times ^1\text{H}$ , C), isotropic g and hyperfine tensors;
<b>‘Spin triplet’</b>	spin system: $S=1$ ; isotropic g; Sys.D = [0.15 0.025];
<b>‘Triplet nitrene’</b>	spin system: $S=1$ ; isotropic g; Sys.D = [1.369 0.093]; W-band;
<b>‘Triplet carbene’</b>	spin system: $S=1$ ; isotropic g; Sys.D = [0.4089 0.093]; X-band;
<b>‘Mn(III) ion’</b>	spin system: $S=2$ ; 1 nucleus ( $^{55}\text{Mn}$ ), anisotropic g-tensor, ZFS;
<b>‘Fe(III) ion’</b>	spin system: $S=2.5$ ; $g=2$ , ZFS;

## Control panel

The **'START'** button runs the calculations and plots energy level diagram and simulated EPR spectra, both the absorption and CW.



Note that the energy level diagram is calculated only for the orientation listed in the experimental panel, if the orientation is not given – it takes default values [0 0 0].

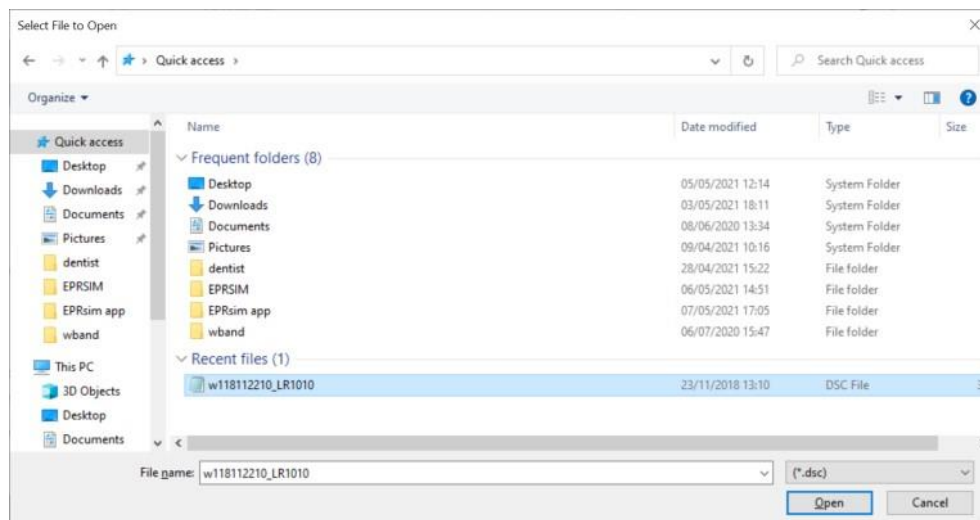
There are also two additional options that can be switched **ON** and **OFF**:

**'SINGLE ORIENTATION'** when selected – the program calculates spectrum of only one orientation as opposed to the whole powder spectrum. This could be used for simulating single crystal type EPR spectra.

**'OVERLAY RESULTS'** when selected this retains previously calculated spectra on the plot. This mode is useful for making figures with several single orientation spectra or when you wish to compare energy level diagrams for different resonance frequencies or orientations.

## Loading experimental data

To load an experimental data file select the **FILE -> LOAD** menu. Select the desired **\*.DSC** file and click the **OPEN** button.



## Saving parameters to a file

To save your parameters as a structure, select the **FILE -> SAVE** menu. All the spin, experimental and computational parameters will be then saved to the specified **\*.MAT** file, which can be used to import those into **MATLAB** environment for further calculations.

