RelaxIS 3 – Advanced Tutorial

Contents of this Tutorial

In this tutorial you will learn the following steps:

- Loading a RelaxIS project folder
- Navigating multiple projects in the same folder
- Data-Validation using the Kramers-Kronig test
- Advanced initialization methods for fit parameters
- Exporting data into spreadsheets and reports

Please follow the steps in this tutorial to learn more advanced features of RelaxIS. Please install and start RelaxIS 3 to begin.

Step 1 Open the Project Folder

On the Welcome Screen click "**Open project folder**" or, if you deactivated the Welcome Screen, choose **Main > Project Folder > Open** from the ribbon bar.

In the Filename field, enter: **%relaxis_appdata%\Tutorials\Advanced** and press *Enter*.

Select **AdvancedTutorialData.eis3** and click Open.
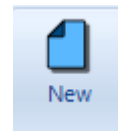
Step 2 – Navigating different projects

The project folder contains two different projects. Too navigate between them use the **Main > Project Folder > Manage Projects** button.

In the management dialog you can add or remove projects by using the + and – buttons, and you can edit the title and description for existing ones.

To continue, please select the **Data Part 2** project and click on **Switch Project**.
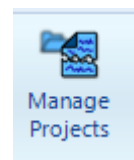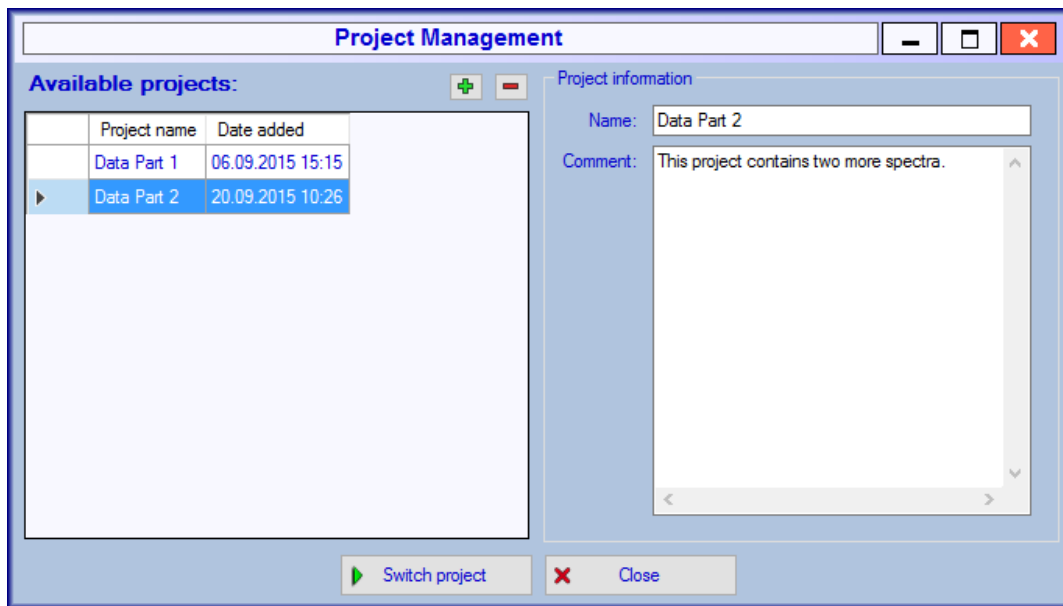
Step 3 – Performing Kramers-Kronig-Tests

- Select the "Multiple Semicircles" dataset.
- Click the **Data and Quality > Data Quality > Kramers-Kronig-Test** button.
- Use the plots to inspect how well the simulated curve reflects the measured data.
  → In this dataset the simulation perfectly overlaps the data. It is therefore very trustworthy data.
- Close the Kramers-Kronig-Test dialog.

- Select the "Randles-Circuit" dataset
- Click the **Data and Quality > Data Quality > Kramers-Kronig-Test** button.
- Use the plots to inspect how well the simulated curve reflects the measured data.
  → In this dataset the overlap in the low-frequency domain is only good if a series capacitance is fitted in the complex fit, due to the Warburg behavior. Play with the settings to see the differences.
- Close the Kramers-Kronig dialog to continue.

Step 4 – Initializing the Fit Parameters using Shapes

Drawing the shapes

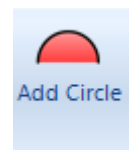Select the "Multiple Semicircles" dataset. Assign this spectrum to the model

> **R-(R)(P)-(R)(P)**
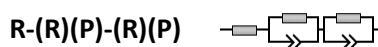
Please refer to the Basic Tutorial or the manual if you are unsure how to do this.

Click the **Fitting > Parameter Helpers > Add Circle** button.

Click & drag anywhere in the Data Explorer graph and notice the circle that appears. The position of the circle is not critical at first. Release the mouse button and click & drag the blue arrows on the circle to position the red circle shape on the left semicircle of the data.

You can **delete shapes** by right-clicking on one of the blue handles on the shape.

Repeat this to place another red circle on the right semicircle of the data.
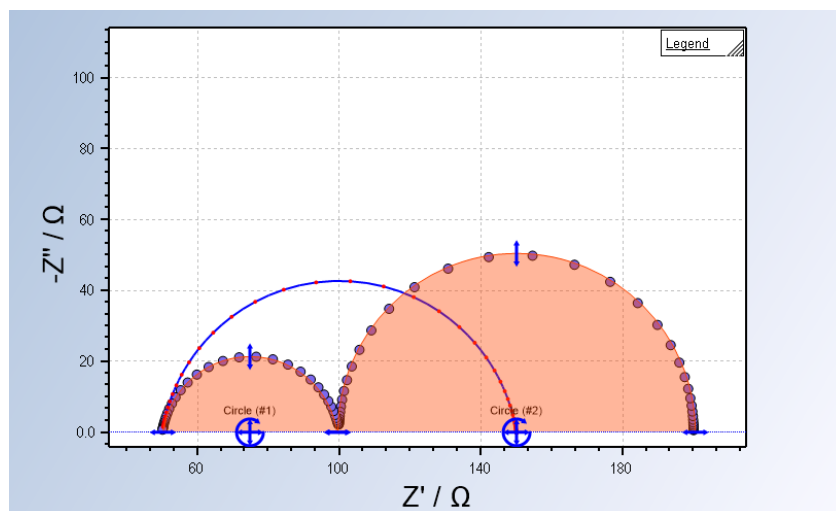
Calculating initial parameters for the shapes

In the Parameter Explorer window you can notice the symbols at the top representing the shapes you have drawn before.

- Click and hold the left mouse-button on the symbol "Circle (#1)".
- Drag the mouse into the parameter list below.
- Notice the green arrows appearing at Resistance/CPE-Q/CPE-Alpha combinations.
- While still holding the left mouse-button move the mouse cursor onto "Resistance 2".
- Release the mouse-button.
- Notice the new values that were calculated for the three parameters (that were indicated by the green arrows).

Repeat these steps to assign "Circle (#2)" to Resistance 3, CPE Q 2 and CPE Alpha 2.

Notice that the blue curve already seems to nearly fit the data. The fit is now initialized very well and you can fit the spectrum.

Using the Line Tool

Navigate to the "Unassigned Files" group using the combobox in the Spectra Explorer window and find the "Randles-Circuit" dataset.

Assign this dataset to the circuit

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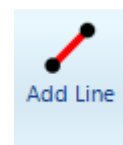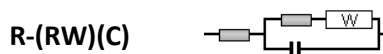
Add a red circle fitting the semi-circle in the data.

Now click the **Fitting > Parameter Helpers > Add Line** button. Similar to drawing a circle, draw a line that fits the linear low-frequency part of the spectrum.

In the Parameter Explorer window drag the "Line (#2)" symbol into the parameter list and release it on "Warburg Coeff. 1".

Also, drag "Circle (#1)" into the list so it marks "Resistance 2" and "Capacitance 1".

Notice, that this fit is now also initialized very well.

Step 6 – Using the Genetic Algorithm to Perform a Fit

Navigate to the "Unassigned Spectra" model using the combobox in the Spectra Explorer window and find the "Complex Data" dataset.

Assign this dataset to the circuit

R-(C)(Ws)-Wo

Click the lower part of the **Fitting > Perform Fits > Auto Fit** button and select **Advanced Search**.

In the Genetic Algorithm dialog click the **Start** button and wait for the algorithm to converge. The *Best Fitness* value should be well below 10^{-20} in this example.
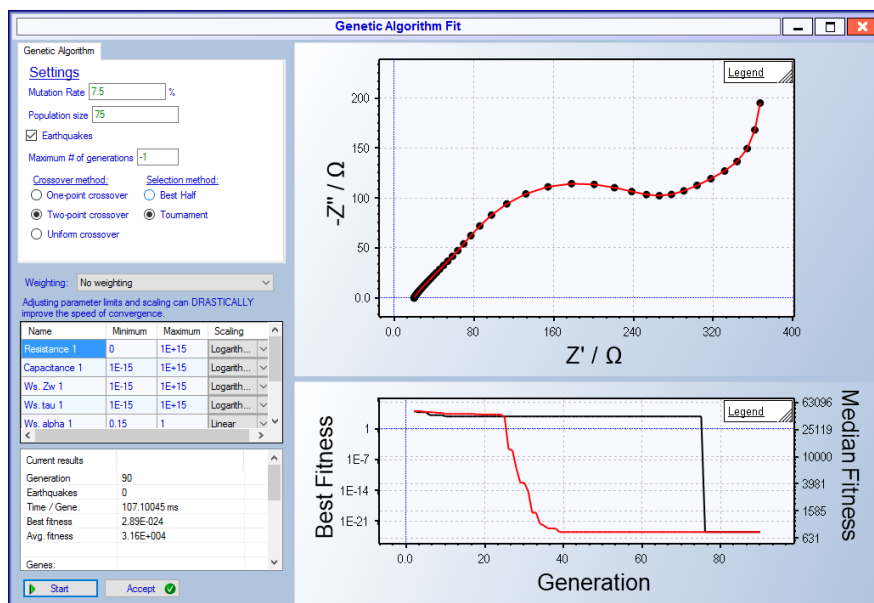
You can also experiment with altering the Minimum and Maximum values for the parameters and watch the effect on the speed of convergence.

When you are satisfied with the results, please click the **Accept** button, which enters the found parameters as initial parameters for the spectrum and performs a Single Fit.

Click on the lower part of the **Fitting > Perform Fits > Auto Fit** button and select **Single Quick** or **Thorough** to perform an Auto Fit of the spectrum, which will run the Genetic Algorithm with default settings and thus automatically fits the spectrum. Compare the non-deterministic nature of the fit, meaning that it may not work well sometimes, with the Thorough fit having a higher success rate.

Step 7 – Exporting Data into Spreadsheets

- Click the **Main > Export Functions > Export Center** button.
- Select **Spectrum Export** and click "File Selection".
- Select "Current Group" and click **OK**.
- In the Select transfer function dialog, select "Impedance" and click **Next**.
- Exclude "All fit frequencies", "All fit real parts" and "All fit imag. parts".
- Click "To clipboard" and paste the data into e.g. Notepad, Excel or another program of your choice.
- The other exporters work in a similar fashion.

Step 8 – Creating Reports

- Click the **Main > Export Functions > Create Report** button.
- Select the *RelaxIS General* template from the list and click **Select template**.
- In the Spectra Selection dialog, choose *All spectra* and click **OK**.
- Browse to a location of your choice on your hard-drive and enter a filename for the report, e.g. *TutorialResults.html* and click **Save**.
- The report is now created and displayed in your default web-browser. You can use any PDF-printing software to convert the HTML-document into a PDF if you like.

Summary

You have learned how to open an existing project folder and navigate the projects contained in it.

You have seen how you can use the Kramers-Kronig-Test to test the validity of the data on two different example spectra.

Afterwards you have used different initialization methods, namely drawing shapes and using the Genetic Algorithm, to initialize and fit various sets of data.

In the last step you have learned how to export raw data into other software and how you can create reports to easily visualize your fit results.