RI Retrieval In Labview

User Manual

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Introduction

This software retrieves the real and imaginary part of a material’s refractive index for multiple wavelengths. It accomplishes this by best fitting theoretical (Mie theory) extinction cross sections including multiple charge contributions to measured extinction cross sections for a number of size parameters. The best fit procedure of minimizing chi squared enables us to predict the estimated uncertainty (one standard deviation) in both the real and imaginary best fit parameters. The users can also select which size will be included in the curve fit, decide if they want to restrict the search to positive real part, and to incorporate extinction or/and diameter factor to correct for invalid calibration.

Installation

Simply run setup.exe and follow through with the installation wizard. The application was built for 1920x1080 screen resolution, anything smaller than that will show a truncated window and may render the application unusable.

Basic Usage

1. Locate the executable RI Retrieval in Labview.exe and double click it. You will the a window as is shown in Figure 1. Please disregard all data that is shown in windows. It will be updated with your measurements later on.
2. Choose Extinction Cross Section File (format is given in the appendix) using the browse button, Shown in Figure 2. This will update both the diameter list shown on the left and the extinction data graph on the right. It will also update the list of available wavelengths.
3. Choose a multiple charge data file. A corresponding distribution graph will be updated on the right. These two files can be generated in IGOR script written by Michel.
4. Wavelength range is automatically selected to include all wavelengths in file. You can choose to minimize the range and even select just a single wavelength by choosing the same wavelength in both the minimum and maximum selections.
5. For basic usage, leave Use Factors uncheck, as it is by default. I will devote a separate section that is relevant to this option.
6. Choose if you want to add error calculation for the parameter estimations. If you want just a rough estimation for the errors you can choose approximate errors. (explanation between the two is given in the appendix)
7. Choose whether or not to restrict the retrieval to positive imaginary values. (Restricted by default)
8. Choose which sizes you want to include in your retrieval by checking the relevant check boxes. I will explain later the usage of the quick fit button. For now, simply leave it off (It is off by default)
9. Press the Retrieve RI button to begin retrieving real and imaginary parts from you data. The button caption will change to “Running..” and return to “Retrieve RI” once the retrieval is done. During the run the following graphs will update in real time: the real and imaginary graph as a function of wavelength (take care not to move the cursors while the program retrieves the data – It doesn’t work because of my program architecture). A blue square will appear if the residue for that fit was less than 3, signifying a good fit. Normalized residuals ((observed-fitted)/uncertainty)) graph as a function of size parameter, Measured data and best fit result as a function of size parameter, and a convergence graph which shows how the algorithm converges to the minimum Chi^2 in the Chi^2 surface (Simplex Algorithm) – all shown in Figure 3. You can only stop the retrieval process by pressing the stop button located at the top of the window.
10. Once the retrieval is finished you can save the data by pressing the “Save RI to file”. A file with the retrieved data will be created in the same directory from which you loaded the extinction file and will be named by the same name plus descriptors of which options were selected to achieve that result.
11. You can also examine the data by moving the cursors in the real and imaginary graph to the desired wavelength. The corresponding graphs and results will be updated. The main result shown in figure 4 – the wavelength and the corresponding real and imaginary parts are shown in the graph. Residue (MDBF) is the calculated Chi^2 divided by number of sizes in between the best fit result and the measured data. Residue (CDMRI) is the calculated Chi^2 divided by number of sizes in between the calculated Mie curve and the corrected for multiple charges measured data.

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| Figure 1 – Main Application Window |

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| Figure 2 – Input data files and choose parameter for the RI retrieval run |
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| Figure 3 – Graphs that update during the retrieval process. (please don’t manipulate the cursors which the retrieval is running) |

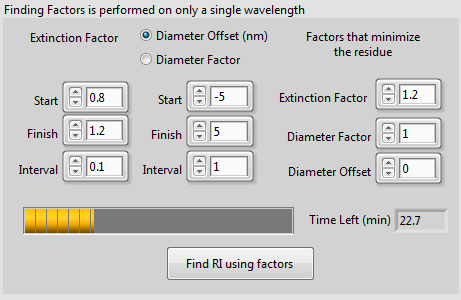
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| Figure 4 – Retrieval results |
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Additional functionality

Fixing calibration errors

If working under the assumption that there can be only Mie curve that can fit the data with a minimum Chi^2, one can calculate the Chi^2 minimum as a function of extinction factor and/or diameter offset/factor and find the minimum minimum Chi^2. The factors the give the above are the calibration factors needed for a successful retrieval. By extinction factor I mean that I multiply the resultant theoretical cross-section by that factor for all sizes. The same explanation goes for the diameter factor. In Diameter offset, I add these offsets to the corresponding diameter sizes before running the calculation.

The scheme provided in the figure below enables the user to select the grid search parameters. If an iteration on only the extinction factor is required then set the start and finish for the diameter offset/factor to the same number. Remember to select a single wavelength and press the button “Find RI using factors” to start the search for minimum of minimums of Chi^2. When the calculation finishes, it outputs the extinction and diameter offset/factors to the third column “Factors that minimize the residue” and automatically calculates the retrieval for those factors. If one then wants to use these factors regularly, he can turn on the “Use Factors” button mentioned previously.



Quick fit function

For the purposes of examining if a single or more sizes were part of bad measurements, I added the quick fit function. The way we suggest to use is as follows:

1. 1. Select a single wavelength
2. Enable the quick fit button, located above the diameter sizes checkboxes.
3. Every time that you select or deselect a size, the retrieval process is run automatically and enables to see how the omission of one or more sizes affected the retrieval results. So, this is in fact to test the robustness of the retrieval process.

Adding a theoretical Mie curve in an arbitrary real and imaginary parts

Choosing whether to fit extinction or absorption data

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| C:\Users\Weizmann\AppData\Local\Temp\VMwareDnD\713799b0\2012-07-09 15.51.47.jpg |
| Figure 5 – Hg and Ar spectral lines |
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Appendix

Format of Extinction file

Format for multiple charge size distribution file

Explanation on how the errors are calculated and what does it mean to approximate the errors

Credits for software

National Instruments - Labview

JKI state machine framework

Mie code dll for labview implementation by …

Simplex algorithm written in labview by ….

Credit to my self