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. Examining the data is done by moving the cursors in the real and imaginary graphs 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) |

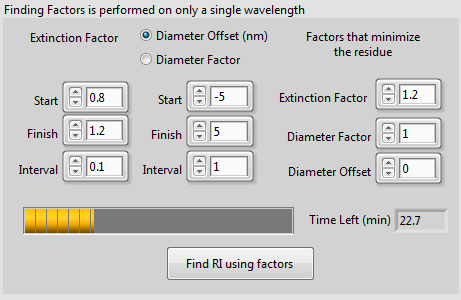
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| Figure 4 – Retrieval results |
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Additional functionality

Fixing calibration errors

If working under the assumption that there can be only one 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 that give the above are the calibration factors needed for a successful retrieval. Extinction factor definition is multiplying 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 is done only on the extinction factor, then to disable the diameter offsest/factor, set its start and finish 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

The quick fit, when enabled, calculates the retrieval immediately after selecting of deselecting a single size from the list. Use this function to check the sensitivity of the retrieval to one data point. These are the recommended steps:

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 ran automatically and enables to see how the omission of one or more sizes affected the retrieval results. So, this is in fact a way to test the robustness of the retrieval process.

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

To add a theoretical Mie curve, which is based on delta function size parameters, choose the real and imaginary parts and press “Append Mie” button. A black line will appear the result graph to the right. It is possible to add multiple lines, which will disappear, upon a new retrieval or if the cursors are moved in the Real or Imaginary graphs. The residue is calculated relative to the Corrected data results (black diamonds).

This function is useful to test if the error estimation was reasonable, or see how far your results were from a specific standard, or to test by how much the Mie curve change when slightly changing the RI’s and in infer your potential retrieval success.

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Choosing whether to fit extinction or absorption data

The possibility of analyzing absorption or scattering cross-section is also added. Select, using the handle, which of the three, extinction, absorption, or scattering cross-section, you wish with to retrieve the RI’ for.

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Appendix

Format for the Extinction file

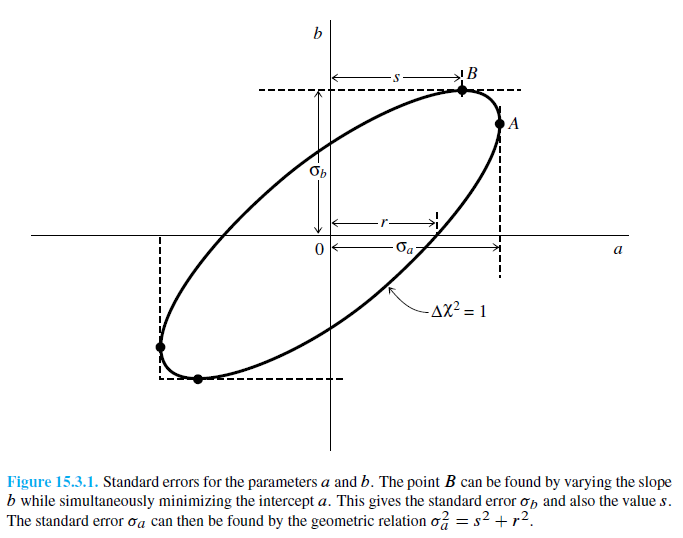
The extinction file is generated by an IGOR script. In principle, one can build the file independently. The file has txt extension and purely tab delimited. Example on how to read the file: The extinction cross-section in cell B4 is measured for a particle size of 241 nm in 365.01 nm wavelength and its uncertainty is given in cell B14.

Format for multiple charge size distribution file

This file is also tab delimited and has a txt extension. The columns correspond to the selected sizes that appear in the extinction cross section file and appear in the same order from left to right. The first column represent the sizes from the SMPS run and the content of the file is the fractional concentration for every size when selecting a single size with the DMA. This of course includes the bigger diameter particles that come from the multiple charging effects.

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

The errors calculation method is described in “Numerical Rescipes in C++ second edition by Press et al.” in chapter 15 Modeling of Data. σ­a and σ­b are the uncertainty calculations done when choosing the “Calculate Errors” option. Choosing “Approximate Errors” calculates the “r” value shown in the figure below, which is taken from Numerical Recipes book without permission (since this is not a published user manual).



Credits for software

National Instruments – Labview

[http://www.ni.com](http://www.ni.com/)

JKI state machine framework

<http://jki.net/state-machine>

Mie code dll for labview implementation by …

Mie scattering demo program, August 2005, by Martin Fierz (martin@fierz.ch)

mie2.dll uses P.J. Flatau's C version of the Bohren and Huffman code

I could not have made this dll for LabView without his work.

In his credits, Flatau writes

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Original program taken from Bohren and Huffman (1983), Appendix A

Modified by B.T.Draine, Princeton Univ. Obs., 90/10/26

in order to compute <cos(theta)>

This code was translatted to C by P. J. Flatau Feb 1998. The C

version uses "Numerical Recipes" public domain code for complex

arithmetics "complex.c" and "nrutil.c" (http://www.nr.com).

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Simplex algorithm written in labview by ….

Laurent Kneip

<http://www.laurentkneip.de/DS.html>

Laurent Kneip  
ANU College of Engineering & Computer Science

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