ICEMAN Tutorial

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Chapter 1

Installation

Before beginning the tutorial, you will need to install Docker and ICEMAN. It is assumed you will already have installed Docker before the tutorial begins. If not, you will only be able to follow along with the tutorial on the screen instead of with your own machine.

1.1 Installing Docker

1.1.1 Mac and Linux

Installation for Mac or Linux machines is straightforward. Simply go to the appropriate link below and follow the instructions.

Docker for Mac (https://docs.docker.com/docker-for-mac/install/)

Docker for CentOS (https://docs.docker.com/install/linux/docker-ce/centos/)

Docker for Debian (https://docs.docker.com/install/linux/docker-ce/debian/)

Docker for Fedora (https://docs.docker.com/install/linux/docker-ce/fedora/)

Docker for Ubuntu (https://docs.docker.com/install/linux/docker-ce/ubuntu/)

1.1.2 Windows

ICEMAN is not compatible with Docker for Windows. Instead, you will need to install Docker Toolbox from the link below.

Docker Toolbox

Docker Toolbox is not compatible with Hyper-V. If you recieve an error message about Hyper-V, you will need to open Windows Features through the control panel and disable all Hyper V options in it.

1.2 Installing ICEMAN

Once Docker is installed, you can download the ICEMAN tutorial folder from your email and unzip it.

Note that on Windows, you will have to unzip to a folder that is somewhre inside your /Users folder. The desktop is a convienent location.

1.3 Getting Started

To start ICEMAN, open a terminal from your operating system's start menul (Mac and Linux) or the Docker Quickstart Terminal that was installed alongisde Docker Toolbox (Windows). You'll need to navigate to your ICEMAN installation directory. You can find the terminal/prompt's current location by typing "pwd" without the quotes and pressing enter. You can move to other folders by typing "cd ___", filling in the name of a folder in the blank. Typing "cd .." will move you up one folder to the parent folder.

Once your terminal is in the ICEMAN installation folder, type "./ICEMAN-install" and wait for the installation process to finish. Then type "./ICEMAN" or "./ICEMAN-windows" depending on your operating system. For Windows, this will give a message with instructions on how to open ICEMAN. For Windows, you will have to open a command prompt by going to the start menu and typing cmd. In this prompt, type "docker-machine ip default" and press enter. Then take the number that was output and type "./ICEMAN-windows (the number)" and press enter. It will look something like ./ICEMAN-windows 196.68.99.100. This will launch ICEMAN in a web browser. From now on, you can simply navigate to this folder and type "./ICEMAN" to launch the program.

Chapter 2

File Type Conversion

One of the services offerred by ICEMAN is the conversion between file types. This is controlled in the Translation tab that ICEMAN initially opens with.

2.1 Uploading a File

In order to translate a file, you will first have to upload it to ICEMAN. You can drag and drop a file into the input column on the left. Alternatively, you can click the Upload button to open a file browser to select a file from your computer. This same process, of either dragging and dropping or using the upload button, will be used anywhere in ICEMAN where an input file is needed for uploading.

In your ExampleData folder, find Ag5SbS4_PhonDOS.phonon and drag and drop it onto the input list.

2.2 Performing a File Conversion

To convert a file, click it in the list of input files. The middle area of the screen will display a drop down box for the various file types that the selected file can be converted into.

After selecting an output type, there may be additional options displayed in the middle section to allow further customization options to be set.

From the drop down menu, select .aclimax.

Once you have selected all options for your conversion, hit the Convert button at the top of the page to convert the file. The resulting file will appear in the list of output files to the left.

Press the Convert button and wait for the conversion to finish.

You can now select the output file in the output file list on the right. By selecting the file and right clicking, you will get the option to download it. Selecting this option will pop up a window with a download button. Click it to download the file.

Click on the Ag5SbS4_PhonDOS.aclimax file in the output file list. Then left click on it to open a menu. If left clicking does not work, the file is not really selected. Make sure the file is shown in blue, and not just outlined. Click the Download option. Then click the Download button that appears and save the file.

2.3 Cleaning Up

As you use ICEMAN, your installation may become cluttered by many files. To remove them, select the file from the list and hit the delete key on your keyboard. The internal ICEMAN copy of the file will be removed.

In the input file list to the left, select Ag5SbS4_PhonDOS.phonon and press the delete key. Then do the same thing to Ag5SbS4_PhonDOS.aclimax in the output file list to the right. The file lists will now be empty, but you can see that the version of Ag5SbS4_PhonDOS.phonon in your ExampleData folder and the version of Ag5SbS4_PhonDOS.aclimax you downloaded have not been deleted.

Chapter 3

OClimax

OClimax is a neutron modeling code integrated into ICEMAN.

3.1 Configuring OClimax Parameters

The OClimax tab has the controls to set up and execute an OClimax calculation. The tab will be initialized with some default values, but you can also load a pre-existing file. You can drag and drop a .params file into the parameter file list on the left of the screen. Selecting a file in this list will give you the option to load it.

Switch to the OClimax tab in the top row of tabs. Find the Ag5SbS4_PhonDOS.params file in your ExampleData folder. Drag and drop it into the parameter file list on the left. Then click on the file name and select OK on the confirmation window that pops up.

The various controls on the page will allow you to configure the specifics of your execution. Outside of the scientific settings, the top row of controls require a bit of explanation. The Name field has the name of the .params file itself. Editing this will cause your new parameters to be written to a new file, while leaving it the same will overwrite any old files with that name.

Edit the text in the name field to read Ag5SbS4_PhonDOS-Tutorial.

The input file field has a button to select a file. Clicking it will open a window to allow the upload/selection of a data file.

Click the Select button under the Input File label. Drag and drop the Ag5SbS4_PhonDOS.aclimax we made in the previous step to the empty list of files. Then select it in the list and press OK.

The save button will save your current parameters to a .params file. This file will appear in the parameter files list to the left.

Click the save button and note the new Ag5SbS4_PhonDOS-Tutorial.params file in the list to the left.

3.2 Running OClimax

To run OClimax, click the Run button. You will likely be asked if you want to overwrite your current parameter file. You can see the progress of the OClimax job as it runs in the panel at the bottom of the screen.

Click the Run button. A window will pop up asking if you want to overwrite Ag5SbS4_PhonDOS.params. Click OK. Watch the text in the panel at the bottom of the screen and wait for OClimax to finish running.

Your output files will appear in the Output tab. In the file list on the left, they will be under the oclimax folder.

Click the Results tab at the top of the screen. Then click the arrow next to the word OClimax in the file list on the left. You can download files by selecting them and right clicking, as before.

Chapter 4

QClimax

QClimax is a code for performing fittings on neutron scattering data. Internally, it uses lmfit to perform machine learning techniques that optimize the model parameters to fit the data. It offers a variety of options for controlling your fitting procedure.

4.1 Creating an Instrument

The first screen in the QClimax tab is the Data tab. It allows you to set up the instrument(s) you will be performing a fitting for and to provide them with data files. The list on the left will display all existing instruments. Clicking an instrument will open it for editing. The + and x buttons above it will allow you to create new instruments or remove existing ones.

Click on the QClimax tab at the top of the screen. Then click the + button in the upper left. A new instrument, named Instrument1, will appear in the list. Click it to open the instrument editor.

The bar at the top of the screen displays the instrument's name. You can edit it to change the name.

Edit the text at the top of the screen reading Instrument1 to replace it with VISION.

The Resolution File control allows you to set the resolution file for the instrument. Click the Select button to open a window where you can upload or

select a data file. When the file is selected, the list of Q values below it will be populated. You can then check/uncheck the q values to determine which ones you want to use in the fitting.

Click the Select button for the Resolution File. Then find VIS_24931_DAVE.dat in your ExampleData folder. Drag and drop it into the panel in the window that popped up. Then select it from the list and click OK.

In the bottom center is the table of data files. To add a data file, click the Select Data button. You can then upload/select data files for this instrument. To remove a data file, you can click the check box in its row of the table to select it, then click the Remove button. You may also toggle whether you want to specify temperatures. When selected, the column of temperatures will appear. You can double click on a temperature to edit it, and click the save option that appears or press enter to confirm your change.

Click the Select Data button. Then find VIS_24941_DAVE.dat in your ExampleData folder. Drag and drop it into the panel in the window that popped up. Then select it from the list and click OK. Then click the check box titled Specify Temperatures. A new column of temperatures will appear in the table. Double click on the value of 1.0 in the temperature column of the VIS_24941_DAVE.dat to open an editor. Change the number to 150 and press enter to set a temperature for this file.

On the right is the list of functions that are in your model. You can add new functions by clicking the Add Functions button. There are three lists of functions available. The first are the default functions that are built in to QClimax. The second are the custom functions that you have written. The third are shared functions that you have specified for a given execution of QClimax. Select the function you want to add and click OK to add that function to the model for the current instrument. You can also click Write Custom Function to write your own python function. This will appear in the list of Custom Functions.

if you select Create Shared Function, the created function will be able to be shared with other instruments in the same execution. It will appear in the list of Shared Functions from now on.

Click the Select Function button to open the add function window. Select the Linear option from the Default Function list. This will add a linear background to the model. Then go through the same process again, this time adding a Delta function. Repeat again, this time adding a Lorentz.

When a function is added to the model, it appears in the panel to the right. The name is displayed and, in the case of shared functions, can be edited.

Non-shared functions always receive a default name. Following the name is the function type. And following that is the Remove button that will delete this function from the model.

Below that is the table of parameters. Each parameter has a name, a starting value, and, optionally, a minimum and/or maximum value. The three numbers are set up with some default values but are editable by double clicking. You can remove a minimum or maximum by editing them and deleting the value.

Go to the Lorentz1 function's parameter table. Double click on the amp row. Edit the Starting Value to 0.5 and press enter. Then double click the cen row. Delete the numbers for min and max then press enter.

4.2 Setting Constraints

The Fittings tab will allow you to configure the fitting(s) that will be performed during the execution. The list on the left contains each run. The + and x buttons allow you to add a new run, or to remove selected run(s), though you can never remove the last run you have in the list. Clicking on a run's name will open it for editing.

Click the Fittings tab at the top. Then click Run1 in the list.

The run's name will be displayed in the top left, where it can be edited.

Click the text reading Run1 in the top left, and edit it to ConstantValue.

Thescreen will list every parameter for every function in your data and allows you to constrain them. For example, the Single Center button at the top will find all parameters named "cen" and set them to be equal to each other. This is a convienence button for the common task of forcing a single center, but the same thing can be achieved manually.

Click the Single Center button. Notice how the Parameter Lorentz1_cen now has P

$$Delta1\_cen$$

written next to it. This mean that the center of the first Lorentzian is equal to the parameter that is the center of the first Delta function.

You can set your own constraints by clicking the Set Constraint button next to the parameter your want to constrain. This will open a window for editing

constraints. You can write a constraint in the box at the bottom and click OK to set it to the parameter. Constraints are Python statements with some special syntax, but can be thought of as mathematical equations for people not familiar with programming.

Click the Set Constraint button for the Lorentz1 wid parameter. Then type 0.025 into the box and click OK. This will set a constraint of 0.025 to the first Lorentzian's width, ie the first Lorentzian's width will always be exactly equal to the constant 0.025.

In the top left is a table of parameters for use in constraints. To add a new parameter, click the x button. To edit a parameter's name, starting value, min, or max, double click the parameter's row and click Save or press enter when done. You can remove a min or max by simply deleting the value from the cell. To remove a parameter completely, click the check box for its row to select it, then click the x button. On the right is the list of custom constraint functions. You can click the Write custom constraint function button to write your own Pyhton function that will be usable when creating constraints.

Click the + button to create a new run, Run2. Click it in the list and edit the name to ConstantVariable. Click the Set Constraint button for the Lorentz1 wid parameter again. This time, click the + button to add a new parameter. Double click its row in the table and change its Starting Value to 0.025 and its minimum to 0. Then edit the text at the bottom of the window from 0.025 to a. This will set a constant constraint to the Lorentzian, but instead of the width for all Qs being set to exactly 0.025, the value they are set to a single value which will be determined during the minimization.

4.3 Configuring Options

The Options tab allows the setting of msicelaneous options for the QClimax execution. Name sets the value for the execution's name.

Click the button Options tab. Edit the name to Tutorial.

The minimization method drop down box allows the user to set which minimization algorithm will be used for the fitting. The error calculation method drop down box allows the uer to set which error calculation method will be used as a fallback if lmfit's algorithm was not able to calculate errors. The special selection of "None" will mean that QClimax will never attempt to calculate errors on its own. This may cause your data to come back without error measurements. The check box for Force Error Calculation will always apply

QClimax's error calculation, even when lmfit was able to calculate errors during the fitting. The error calculation steps field will allow you to set the number of steps to perform during the error calculation.

In the bottem left, there is a table for setting the energy range for various temperatures. The values outside of this range will be ignored during the fitting. The + button will add a new row to the table. Double clicking on the row will allow you to edit the values. You can click the check boxes in the rows to select them, then click the x button to remove the range restriction.

You can also set a parameter initalization file. These .json files are generated by QClimax and allow you to use the ending values for parameters as the initial parameter values for another, so that you start off the minimization closer to the optimal values.

4.4 Executing QClimax

The Execute tab will allow you to save your QClimax configuration and run the fitting. This can be done with the Save Configuration File and Run buttons. When run, the QClimax job in progress will display in the panel on the screen.

Switch to the Execute tab. Click the Save Configuration File button. Then click the Run button. You'll get a pop up window asking if you want to overwrite Tutorial.ini. Click OK to perform the QClimax job.

4.5 Visualizing Results

You can visualize the results in the Results tab, by finding the output folder inside the QClimax folder and clicking on the .csv file. This will open a file with all the data inside.

Click the Results tab. Click the arrow by qclimax to open the qclimax folder. Then click the arrow by your job's timestamped folder to open it and inspect the output files. Click on VIS_24941_0_.csv to open a graph.

In order to make sense of the data, you will need to set the graphed series to a set that makes sense. To do this, you can right click to open a context menu. The context menu will have options to Set Independent Series (the x axis) and Set Dependent Series (the y axis). Setting the independent series will open a window to select a series. Setting the dependent series wil open a window with

a list of series and an empty list of series to be displayed. You can select which series will be shown by selecting them in the left list and using the arrow buttons to move them into the right list.

Right click the graph and select Set Dependent Series. Select Lorentz1_wid, click the right arrow button to move it to the right panel, and click OK. Right click the graph again and select Set Independent Series. Select Q from the list and press OK. The graph will now display the Lorentzian's width plotted against the Q values.

You can also change the graph to a logarithmic scale to better see the results of the fitting itself. This can be done by right clicking and selecting Edit Y Axis.

Right click the graph and select Set Dependent Series. Select Data, Q1 Delta1, Q1 Lorentz1, and Q1 Linear, click the right arrow button to move them to the right panel, and click OK. Right click the graph again and select Set Independent Series. Select Energy from the list and press OK. Right click again and select Edit Y Axis. Change the Range Min to VALUE, the Range Max to VALUE, and the Axis Type to Log.