QACD-quack Tutorial

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This is a brief text-only tutorial on how to use QACD-quack. It uses the test data that is included with the QACD-quack source code. You should have previously followed the Quick Start Guide which shows you how to obtain QACD-quack and get it running.

To start, `cd` to the directory that you unzipped QACD-quack into, and run it using

```
python quack.py
```

Create new project

1. Select Project | New from the menu.
2. Enter (or select) a name for the project file that will contain all of the project's data. As we are using the supplied test data, a sensible name is `test.quack` – you only need to enter `test` as the `.quack` is automatically added for you. The QACD-quack project file can be anywhere you wish, it doesn't have to be in the same directory as the imported raw data as the project file contains its own copy of the raw data.
3. Click the Save button or press Enter to accept the project file name.
4. Navigate to the directory containing the raw CSV files, which is called test_data. Select all of the CSV files, using a combination of mouse clicks and the shift or control key depending on your Operating System.
5. Click the Open button and the raw data files will be imported. A progress bar is displayed as this occurs, but because the data files are small the import will be very quick.
6. The project file is automatically updated whenever you make any changes, so there is no need for any 'Save' or 'Save as' functionality in the main menu.

View raw data

1. The application window is divided into two sections. In the left section there are a number of tabs (only one is displayed initially) containing lists and/or tables of items that you can select to be displayed in the right section. There are various controls above the right section to alter what is displayed there.
2. Select the first row in the list on the left, corresponding to Al. On the right will be displayed the raw aluminium element map with a histogram underneath. Both the element map and histogram are displayed using the same colourmap. The histogram has 100 bins, and the mean, median and standard deviations are displayed using solid and dashed vertical lines.
3. At the bottom of the application window is a line of text summarising how large the element map is, the number of valid and invalid pixels, and statistics such as minimum, maximum, mean, median and standard deviation.
4. You can choose to display just the element map, just the histogram or both by changing the Plot type in the dropdown box above the plots.

5. When, later on, you have stored one or more phase maps or regions, one of each can be selected in the Phase and Region dropdown boxes above the plots to filter the displayed element map and/or histogram to only include those pixels specified in the selected phase map and/or region.
6. You can zoom in the element map. If you move the cursor over the map it changes to a cross. Click and hold the mouse button to start selecting a zoom region, then move the mouse to select the rectangle of interest and release the mouse button. The element map will zoom to your specified rectangle. The histogram and text at the bottom of the window remain reflecting the statistics of the whole element map rather than the zoomed area shown.
7. You can zoom further, and each zoom rectangle is stored for reuse. Navigate back and forward through the zooms using the Undo and Redo buttons above the plot. If you switch to a new element map, the zoom is retained so that you are looking at exactly the same rectangle each time. This is handy for comparison between different elements, etc.
8. Select a different element in the list on the left and that element map will be displayed on the right using the current zoom level. As well as individual elements, there is a Total of all elements as well.
9. You can sort the items displayed in the list on the left by clicking on one of the column headings.

Display options

1. Select Options | Display… in the menu to look at the various display options available. An extra window is displayed containing two tabs, the first is named Colourmap, the second Labels and scale.
2. Select the Colourmap tab. All of the available colourmaps are displayed. You can choose a new colormap and click the Apply button, or double-click on a colourmap to select it. There is also the option to Reverse the colourmap. The default colourmap is ‘rainbow’.
3. Select the Labels and scale tab. Here there are various options relating to labels and scales, the most important of which is the use of a physical scale rather than pixels. Tick the Use physical scale check box, and specify the size of a pixel in terms of number and units, e.g. 1.2 nm. If you apply this, the axes labels change from pixels to physical units and a scale bar is displayed. The size of the scale bar automatically adjusts to the size of the zoomed area displayed, and the location and colour of the scale bar can be altered.
4. The Display options window can be kept open whilst you select different element maps, zoom in on areas of interest, etc. You can close it by clicking on the Cancel or OK buttons.
5. Display options are saved in the project .quack file and are hence specific to a particular project.

Filter and normalise data

1. Select Action | Filter and Normalise… from the menu.
2. There are two filtering options: clipping pixel totals and 3x3 median filter. By default both are selected. Leave them both selected and click OK.

3. A progress bar is displayed whilst the filtering and normalisation are performed. When completed, six more tabs will appear on the left hand side; only the first two (Filtered and Normalised) contain anything, the other three are initially empty.
4. Click on an element in the Filtered tab. There are white regions corresponding to invalid pixels, i.e. pixels that have been removed by the filtering process. The list of filtered elements includes a Total.
5. Click on an element in the Normalised tab. A normalised element map is the corresponding filtered element map divided by the total filtered map, and hence each pixel is in the range 0 to 1. There is no Total in the Normalised tab as all valid pixels would be 1. There is however a h-factor which is a weighting used when calculating ratios.

Create a preset ratio map

1. Click on the Ratios tab to select it. Initially there are no ratio maps so the list is empty. To create one, click on the New ratio button at the bottom of the tab.
2. A new dialog box is displayed containing two tabs, one for Preset and one for Custom. Keep the Preset tab selected.
3. Under Valid presets there is a list of the presets that are available for this project which is determined by the elements that exist in the project. For this test project the valid presets are anorthite, Cr# and Mg#.
4. Click on one of the available presets. The formula for this preset will be displayed below the list, as well as the name of the preset. You can edit the name if you wish. Ratio map names are unique so you cannot create a new ratio map with the same name as an existing one.
5. Below the name is a list of correction models that can be applied. By default no correction model is selected; you can choose a different one if you wish.
6. Click OK to create the new ratio map.
7. The dialog box will close and the new ratio map will be added to the list on the left. Its name, formula and correction model are displayed.
8. The new ratio map is automatically selected in the list on the left so that it is displayed in the plot on the right.
9. You can change the name of a ratio by double-clicking on it, and you can delete the current selected ratio map by clicking on the Delete ratio button at the bottom of the tab.

Create a custom ratio map

1. Click on the New ratio button at the bottom of the Ratios tab, and select the Custom ratio tab.
2. Here you create a custom ratio by specifying the elements that comprise the ratio. It is possible to create a ratio of 2, 3 or 4 elements. Choose how many elements, e.g. 2, and those elements to use, e.g. Ca and Mg.
3. As you change the elements, the Formula is updated.
4. Enter a unique name to use for this ratio map, and optionally a correction model.

5. Click OK to create the custom ratio map.
6. The new ratio map is added to the list on the left and automatically selected so that it is displayed in the plot on the right.

k-means clustering

1. To perform k-means clustering, select Action | k-means Clustering from the menu.
2. A small dialog box is displayed containing clustering options. You can specify the minimum and maximum number of phases (k), and whether to include all of the elements in the project or just those of the commonest 5 elements (Al, Ca, Fe, Mg, Si) that are present.
3. Click on the OK button to perform clustering. If you have already done this before, a warning will be displayed informing you that this will delete the results of the previous clustering.
4. A progress bar is displayed whilst the clustering is performed. For large datasets (number of pixels and number of elements) this can take quite a while, but is very fast for this small test data set.
5. For each of the k-values, an item is added to the list in the Clusters tab on the left.
6. Select an item in the list on the left, as usual, to display it on the right. The order of clusters that are returned from the k-means clustering algorithm are reorganised in a repeatable way so that the colours used for particular regions of the cluster map should be fairly constant as you change k.

Create phase maps from cluster map

1. Select one of the items in the list on the Clusters tab, and click on the New phase(s) button at the bottom to create phase maps from the chosen cluster map.
2. A new dialog box is displayed showing the cluster map at the top and information about each of the phases below that. Initially the phases are given default names such as <phase 3>; these can be changed by double-clicking on them in the usual manner.
3. It is possible to select multiple phases in the list control. If one or more phases are selected, they can be deleted by clicking on the Delete selected phases button. When this is done, the corresponding pixels are set invalid and are displayed as white, and the statistics under the cluster map are updated to reflect this.
4. If two or more phases are selected at the same time, they can be merged into one by clicking on the Merge selected phases button. The selected phases are then merged together and displayed as a single colour.
5. The fifth column in the list control shows the Original values that comprise a particular phase. Using this information and the value of k, it is possible to reconstruct the phase maps again from scratch at a future date.
6. When you have finished deleting, merging and renaming phases, click on the OK button to create new phase maps.

7. The new phase maps are added to the list in the Phases tab. Select one in the usual manner to display it on the right. A phase map is always displayed as black pixels and without a histogram, regardless of the current Plot type.

Create phase map by thresholding filtered element maps

1. It is also possible to create a phase map by applying thresholds to one or more filtered element maps.
2. In the Phases tab, click on the New phase button at the bottom.
3. A large dialog is displayed containing a filterered element map at the top, a list of elements and thresholds in the middle, and the corresponding phase map, which is initially empty, at the bottom. On the right are sliders to change the thresholds, buttons to update and clear thresholds for the current element, and a text box to enter the phase name.
4. Select an element of interest, such as Na, in the list control in the middle. The filtered Na element map is displayed at the top.
5. The initial values of the sliders are set to reflect the minimum and maximum values in the filtered element map. Hence the initial thresholds are at the extremes of the values shown and no pixels are removed by this thresholding.
6. Move the slider for the Lower threshold upwards until it is about 100. Now pixels with values less than 100 are removed from the filtered element map plot at the top of the screen.
7. Similarly, move the slider for the Upper threshold downwards until it is about 600. Pixels above this threshold are removed from the plot.
8. Whenever either threshold is moved, the colourmap limits are updated to reflect the change so that the whole colourmap is used to display the remaining pixels.
9. Click on the Update button to update the thresholds for this element in the list in the middle of the dialog. The phase map at the bottom will be updated.
10. Thresholds can be applied to more than one element, and the phase map comprises those pixels that are within the thresholds of all elements of interest.
11. Enter a name for this phase map and click on the OK button.
12. The new phase map is added to the list in the Phases tab and it is automatically selected so that it is displayed on the right.

Display element map using a phase map

1. Select, for example, the Normalised tab and click on an element, and select Map and histogram in the Plot type dropdown box.
2. The element map and its histogram are displayed on the right, and the statistics at the bottom of the application window refer to the entire element map.
3. In the Phase dropdown box at the top, select one of the newly created phase maps.

4. The element map and its histogram on the right and the statistics at the bottom of the application window are updated to refer to only those pixels that are in the selected phase map.

Create a region

Regions are user-specified areas of an element map. They are similar to phase maps but are specified geometrically rather than by elemental composition.

1. To create a new region, select Action | New Region from the menu.
2. A dialog box is displayed describing how to create a new region. First choose the shape of the region, either ellipse, polygon or rectangle.
3. Select the area of interest on the currently displayed element map using the mouse. The exact process depends on the shape of the region.
4. For an ellipse or rectangle region, put the mouse at one corner of the area of interest, click and hold the mouse button and then drag the mouse to the other corner of the area of interest. Release the mouse button to complete the region. The region is displayed as you move the mouse, and when the region is completed the pixels that lie outside of the region are displayed more faintly than before.
5. For a polygon region, click the mouse button at each polygon point. Both the points and the lines between them are displayed. To close the polygon, either double-click the mouse button at the last point, or place the mouse over the first point, which will be displayed in yellow, and click the mouse button once. When the region is completed the pixels that lie outside of the region are displayed more faintly than before.
6. Enter a name for the region in the ‘Create new region’ dialog box.
7. Click OK in the ‘Create new region’ dialog box to add the new region. It will be listed in the Regions tab.
8. When you are editing a new region, it is possible to switch to a different element (or ratio, cluster, etc) map in the normal manner.
9. You can display a region by clicking on it in the Regions tab. The pixels included in the region are displayed in black.

Display element map using a region

1. This is achieved in a similar way to displaying an element map using a phase map, but uses the Region dropdown box rather than the Phase dropdown box.
2. It is possible to select both a phase map and a region, and the only pixels displayed will be those that are within both the phase map and the region.