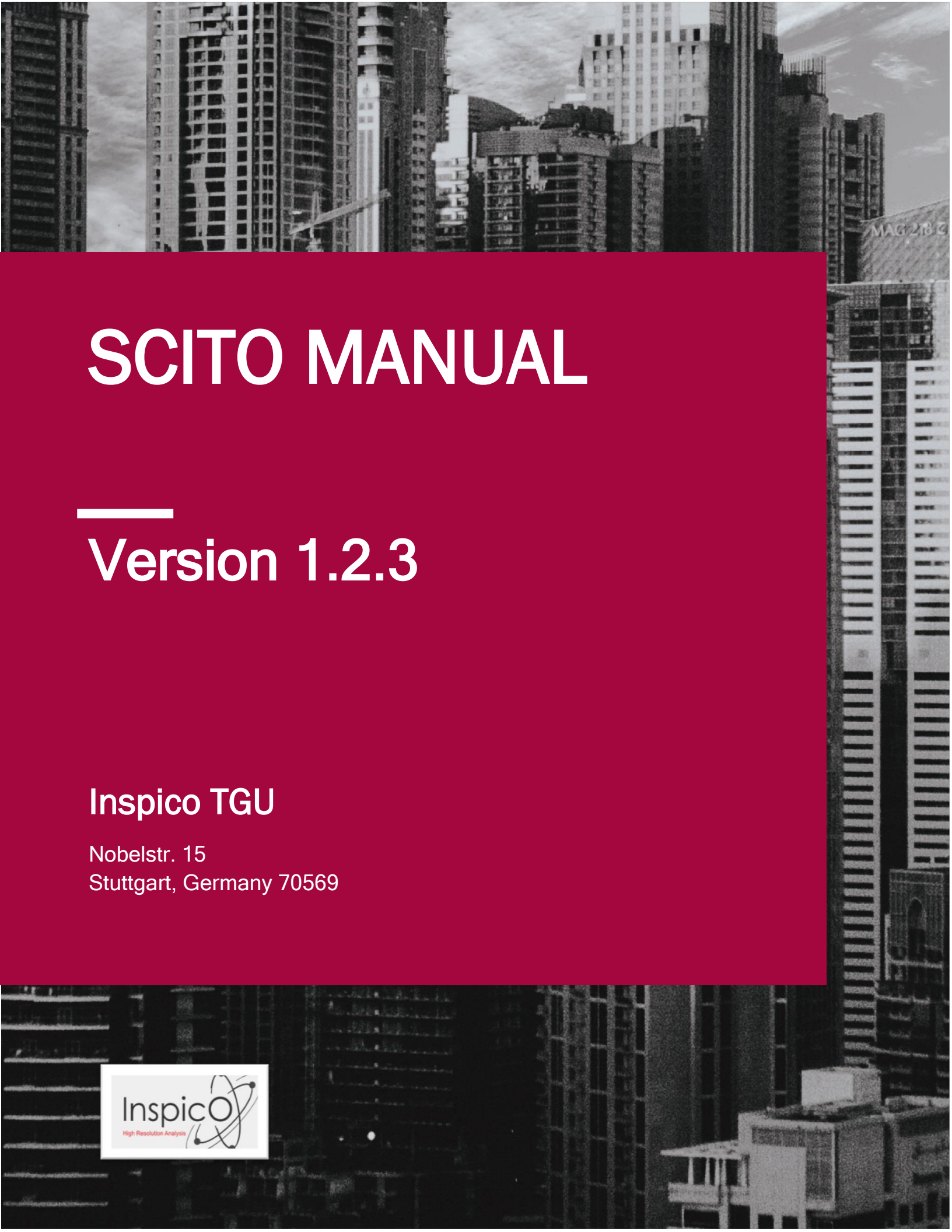

SCITO MANUAL

Version 1.2.3

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Scito Manual

This document is meant to be a starting point on how to use Scito. It is intended to be used as a manual while you are working with Scito and it is prepared to help new user as well as show experienced users deeper functionality.

Overview

With Scito we developed a software that offers extensive functionality while keeping an interface that is user-friendly and gives you the opportunity to fully control what you are doing. Scito consists of several windows (or tabs as we will be calling them) each of which has a unique purpose towards reaching the same goal. In this page we will briefly describe them while in the following pages a more detailed description can be found.

AUTHENTICATOR

First is the authenticator tab which is the first thing that shows up when you run Scito. This tab provides an interface to allow the user to enter his/her login credentials in order to use Scito.

PROJECT

Once authentication is complete the Project tab opens. In this tab you can view information about your project, computer and updates or manage the project you are working on.

MASS

The raw tab gives information on the raw data and also allows for filtering.

RAW

The mass tab shows information about the mass and time-of-flight and allows for modification of the mass windows and calculation of the mass. Also it provides the possibility to modify correction factors.

ALLOY

The alloy tab manages the alloy definition by allowing creation and deletion of elements.

RAW

The reconstruction tab offers different reconstruction algorithms to calculate coordinates in 3D.

RAW

The 3d-View tab is a 3D world that simulates the reconstructed tip allowing for further analysis.

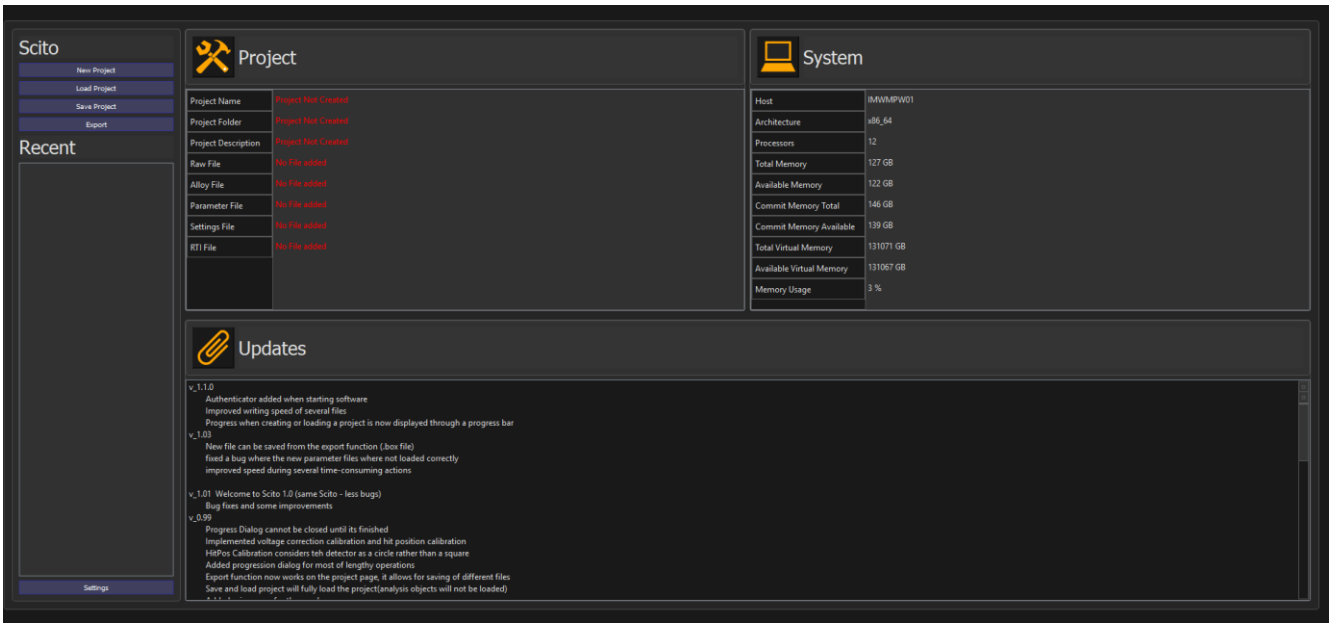
Authenticator Tab

The authenticator Tab provides the means for the user to log in. Upon acquiring a license, a username and a password are generated that allow the user to use Scito. The “Username” and “Password” fields are to be filled with the information received with the license. A network connection is required to authenticate the data provided. The Authenticate button at the bottom is used to submit the data provided and if they are correct then the full functionality of Scito is available to the user.

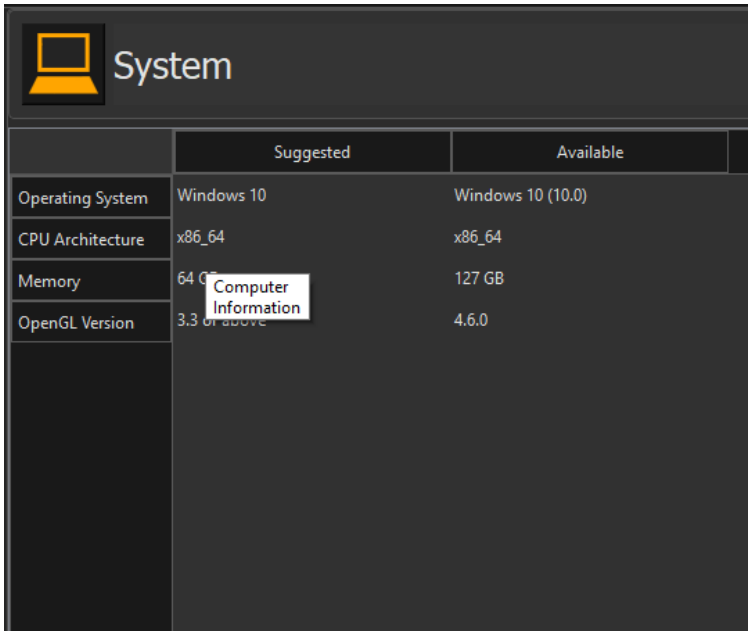
TYPICAL WORKFLOW

Enter Username -> Enter Password -> Press Authenticate

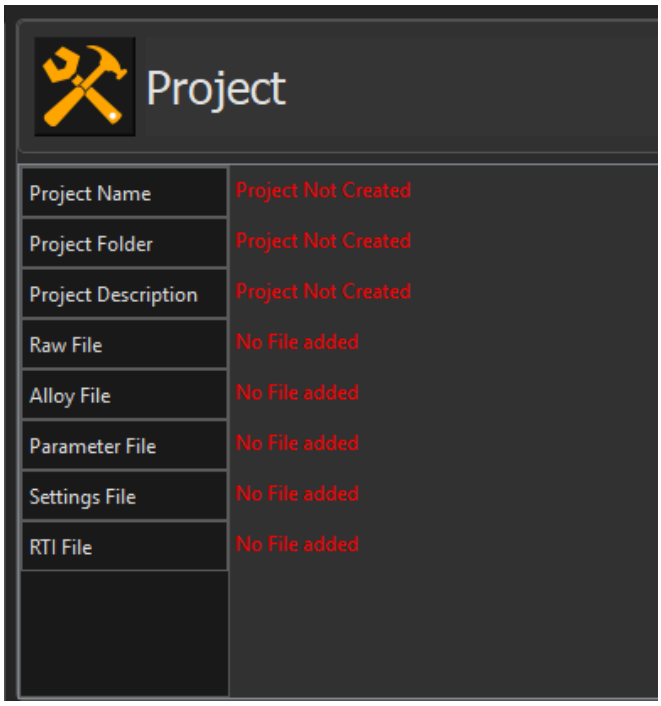
Project Tab



The project tab is where you can create, save and organize your project. The tab is divided in several parts each of which contains different information and allows for actions.



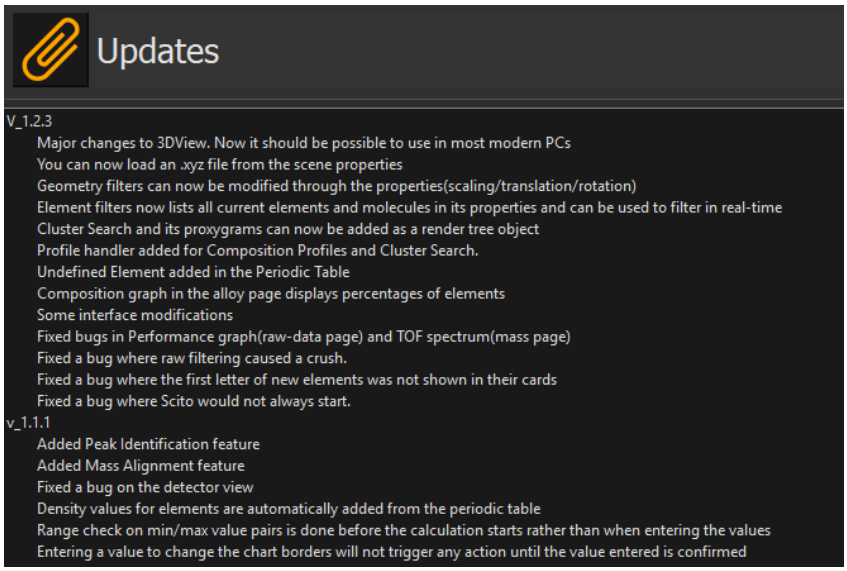
On the top right side information about your computer are displayed. Scito comes with certain computer requirements and this section could be very useful to check those requirements.



On the left of the system information you can find the project information. A project is composed of .pro file and 1 or more other files. The project name is a unique name that you can choose for your project. Ideally you would choose something that can give you an idea of what the project is about. The project folder displays the location where the project lies in your file system. Ideally you would have a central location where you keep all your Scito projects. Project description contains more detailed information about the project which can help you understand what the aim of this project is. A project can contain an additional 5 files alongside the pro file. These are:

- Raw file: it contains data for every event that was detected by the detector. The file is the end result of your measurement and is the main input of your Scito project.
- Alloy File: It contains information about the alloy definition of the project. The content of this file describes how events are distinguished.
- Parameter File: This file contains information on the machine. It should rarely be changed.
- Settings File: contains information about the project that can help you recreate a project when you load at another time
- RTI File: contains information on the tree structure of your 3d view (more on this later).

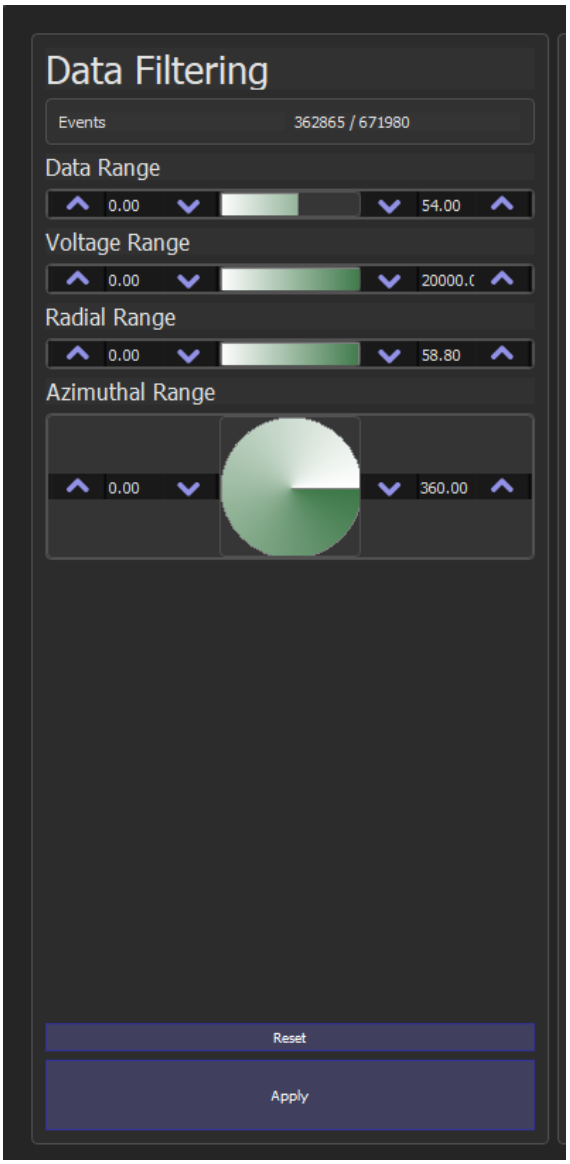
The project can have any number of this files although missing some of them couldn't change the dynamic of your work.



The lower part of the project tab contains a list of recent updates of Scito. When a new update is released the changes are added in this section and the version number increases. More about the updates can be found on our forum.

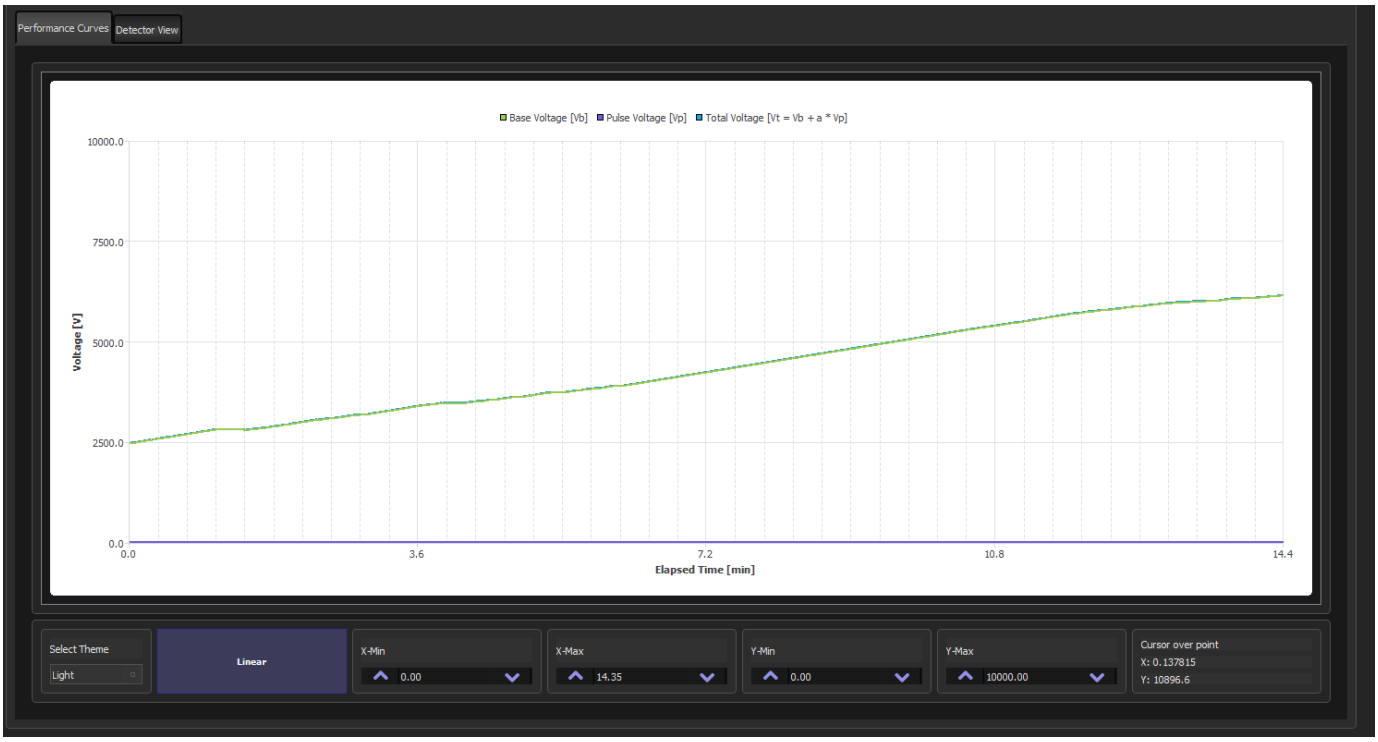
The left part of the tab contains several buttons that serve different functionality.
The New Project button allows you to create a project from scratch. You have the possibility to choose a name, a location and a description for the project. Additionally, you can choose which files you want to add to your project.
Load Project opens up a window where you can search for an already existing pro file which will be loaded to Scito. After saving a project you can use this functionality to load your project to the state that you left it last time that you worked on it.
The Save Project button will automatically create all files of the project using the current information that Scito contains about your project.
Export opens up a window where you can choose what file you want to create (more on the different types of files later).

Raw Tab



The raw tab provides some extra information on your raw data. On the left side there are some filtering options that you can choose. On top it shows you the current number of events after filtering and the total number of events. There are 4 different types of filters that you can use.
The data range filter filters the events based on the order that they are recorded. You can choose the percentages on the left and the right or just move the bar in the middle by holding the left mouse button, and the range you chose is what will be kept, the rest is filtered out. In this case, the first 54% of the events are kept.
The voltage range filters event based on the voltage that they were recorded on.
The radial range offers filtering based on the distance of the position where the event was recorded on the detector, from the center of the detector.
The azimuthal uses the angle of the position of the event on the detector so that you can choose “a piece of the pie”.
You can choose multiple filters at once and to apply them press the Apply button at the bottom. The reset button will remove all filters.

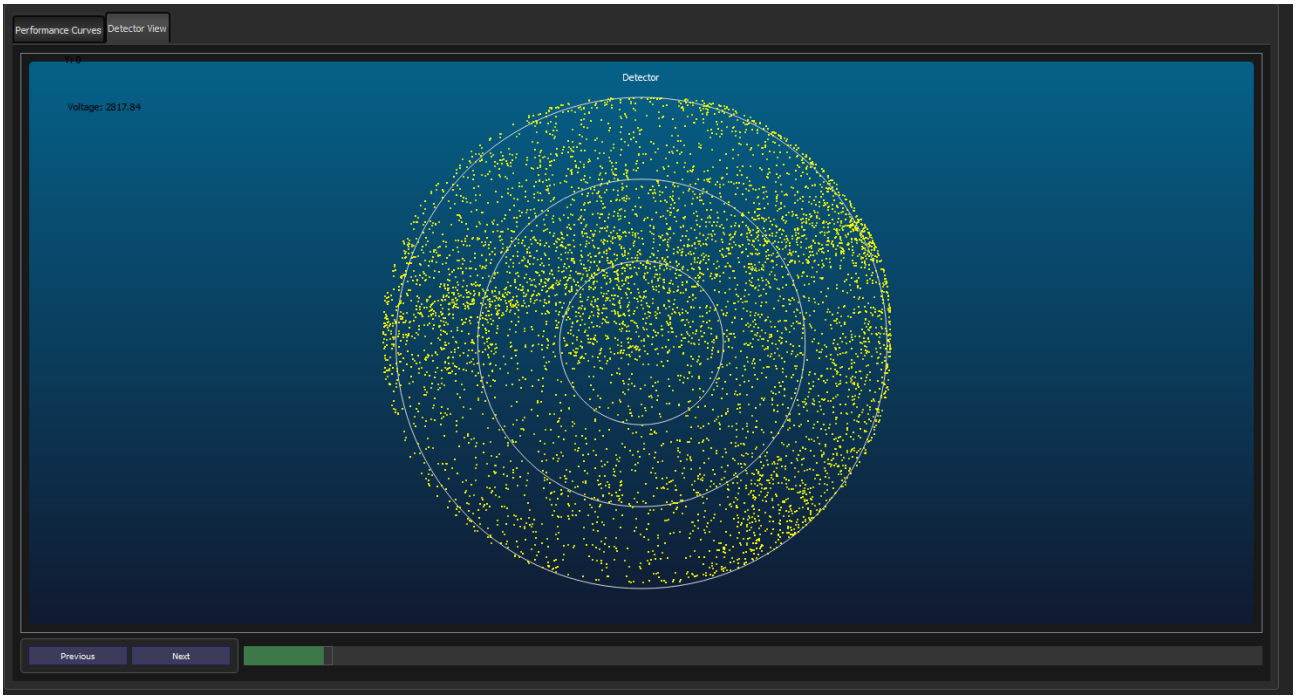
The majority of the raw tab contains 2 charts.



The button on top allow you to switch between the two. The performance chart shows how the voltage changes over time. The controllers for the chart are on the bottom. From left to right their functionality is as follows:

- Left most: choose the theme of the graph. This will change the colors of the chart.
- Second button allows you to switch between a linear and a log chart.
- The next 4 controllers set the minimum and maximum of the 2 axes.
- Right most shows the coordinates where of the position of the mouse.

Most of the charts use this same structure. For more shortcuts on the chart check the Shortcuts section of this manual.



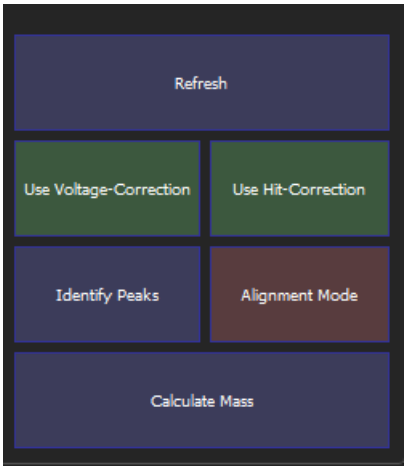
The detector view shows the exact position on the detector where each event was detected. The bar at the bottom can be moved to show a different point in time. Every time point contains 3000 events and on the top left you can see the average voltage of these events.
Once a filter is applied both charts will be updated to display the new information.

Mass Tab

The Mass Tab consists of 4 sections: Mass-Spectrum, Time-Of-Flight Spectrum, Voltage Correction and Hit-Position Correction. The sections are designed to work independently but they also share information

Mass Spectrum

When clicking on the Mass Tab an empty Mass Spectrum page is first opened. On the left side there are some parameters that are needed to calculate the mass of every event.



On the lower part there are several buttons:

Refresh: Calculates the Mass-Spectrum and also updates the Mass Windows.

Use Voltage Correction: When green the voltage correction factors are used on the masses.

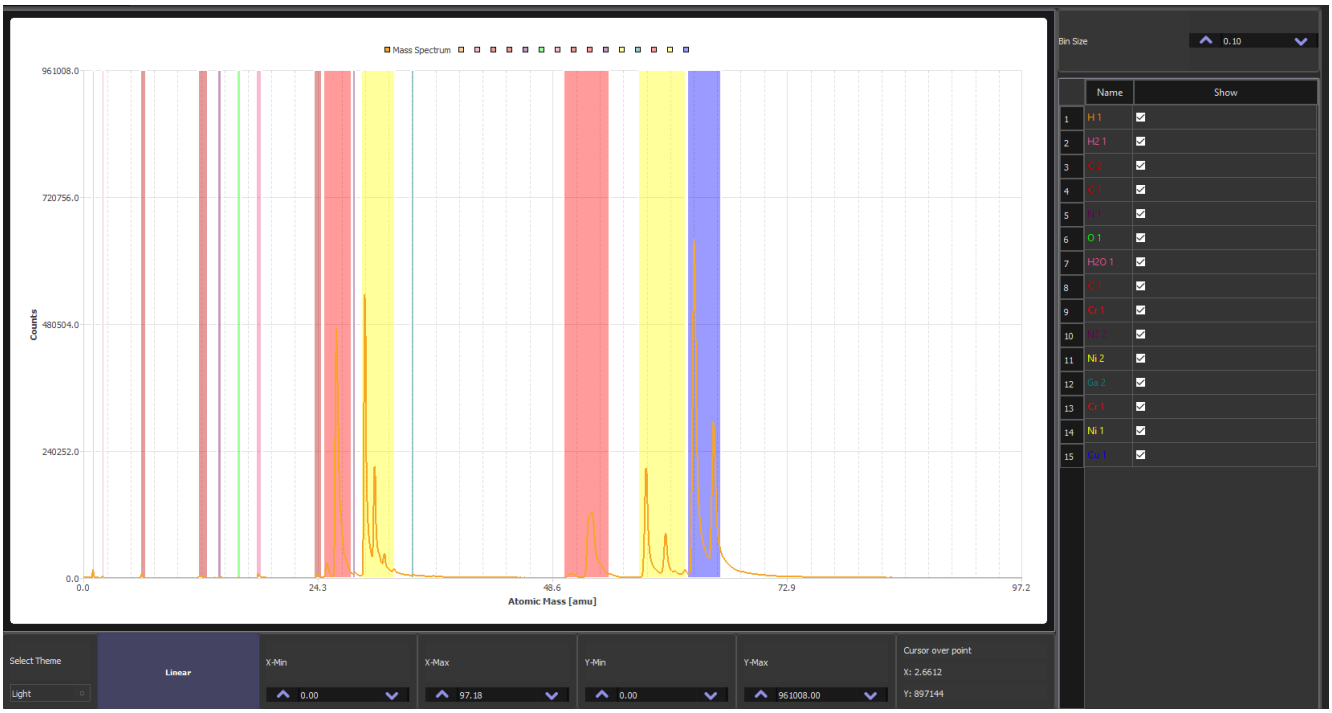
Use Hit-Correction: When green the Hit-Position correction factors are used on the masses.

Identify Peaks opens the Peak Identification window.

Alignment Mode: When green you can aling peaks to a certain position.

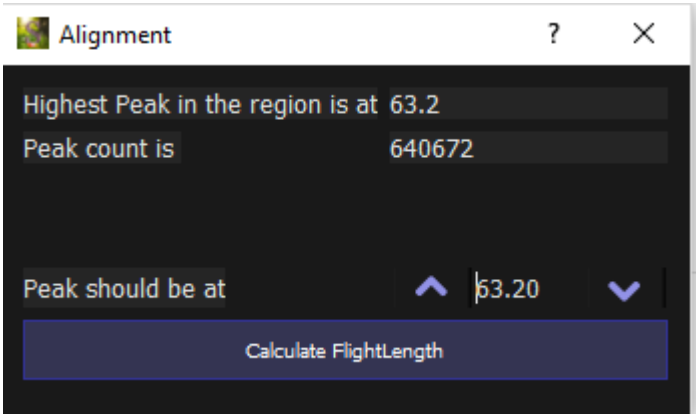
Calculate Mass: Calculates the mass of every event and creates a Mass Spectrum Chart which is displayed in the center of the screen. Also if there

are any Mass Windows loaded with the project they are listed on the right side of the screen. The picture below show how these looks.



Here you can modify the Mass Window ranges using simple mouse controls as follows.

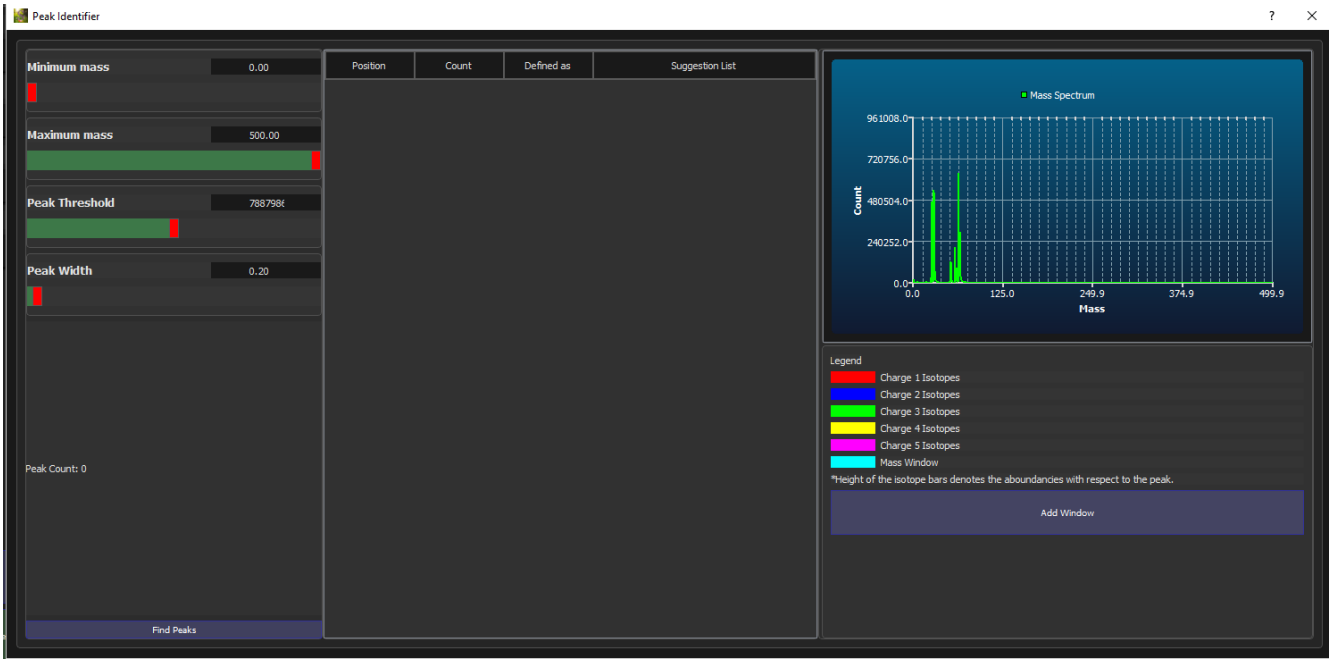
- You can select a mass window by clicking on its name in the table on the right or by left clicking on its region on the chart
- You can move a mass window by holding the middle mouse button (scroll bar) and moving the mouse to the desired position.
- You can move the borders of a mass window by holding the right mouse button and moving the desired border to the new position
- In order to move the mass window or any of its borders a mass window needs to first be selected.



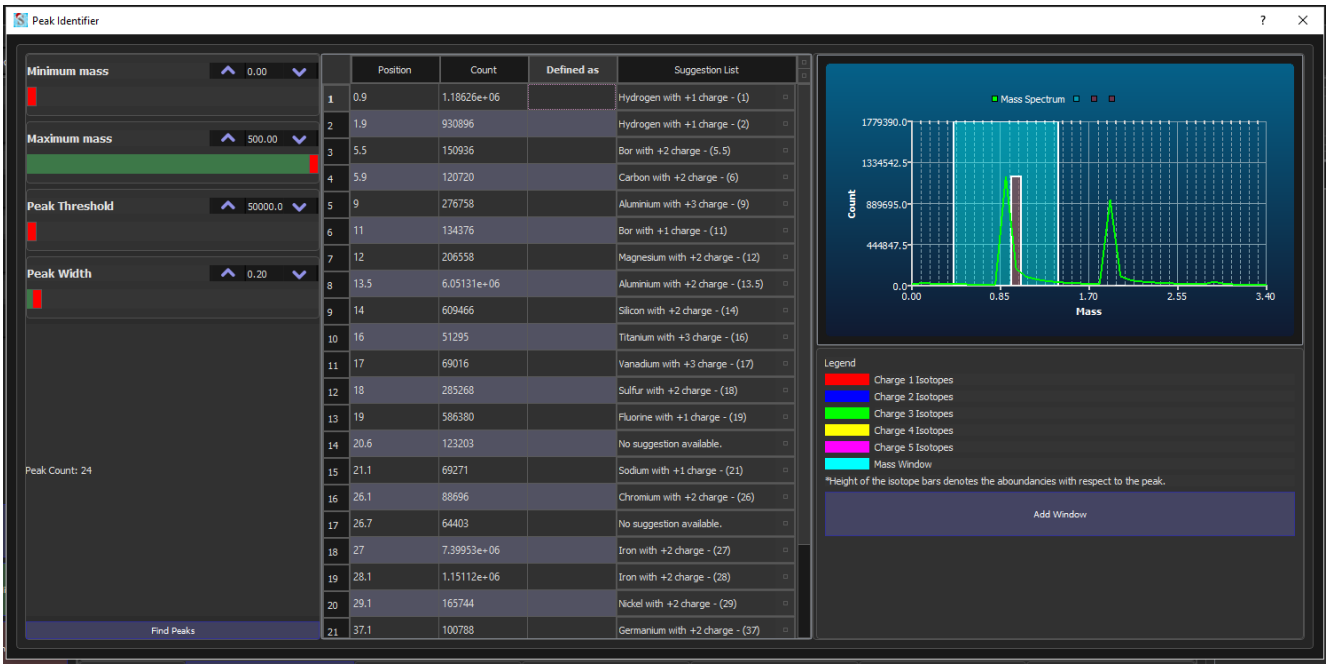
Clicking Alignment Mode will change the color of the background of the button to green and change the cursor to a crosshair. Then clicking anywhere on the mass spectrum will find the highest pek around the cursor and open the Alignment window.

Here you are shown the position of the peak and how high it is. You have to enter the correct value where that peak should be and click Calculate FlightLength. Keeping the Time Offset constant the Flightlength will be adjusted to send the peak to the position specified. Then the mass spectrum is recalculated using the new values.

Clicking the Identify Peaks button will open the Peak Identifier window.
On the left side there are several option for choosing how to calculate the peaks. This feature gives suggestion for what different peaks can be. The suggestion at the moment are only possible for elements and not molecules.



Minimum and maximum mass will cut the mass spectrum and search for peaks in the region specified.
Peak Threshold defines what is a peak. In order for a point to be considered a peak its count should be higher than this threshold.
The Peak Width can be considered as an error margin. Since peak might be slightly shifted from their textbook position (due to calculation or correction errors), increasing this value helps get more suggestion even if the peak is not in the correct position. Lowering this value will give you less but more accurate suggestions.



Clicking the Find Peaks button a list of peaks (their poistion and height), what are they currently defined as according to your existing alloy definition and a suggestion list will be displayed. Selecting one of them on the table will display a zoomed in mass spectrum on the right side with all the isotopes as weighted bars. The height of the bars shows the abundance levels of the different isotopes.
The possible suggestion list contains a list and changing the selected suggestion will update the mass spectrum. The blue window in the mass spectrum can be modified using the same controls as the mass windows on the Mass page.
To move the border of the chart the following hidden controls can be used.
Left and Right keys will move the right border.
Up and Down keys will move the top border.

Holding down the Shift button while pressing the Left/Right or Up/Down key will move the Left and Down borders respectively.

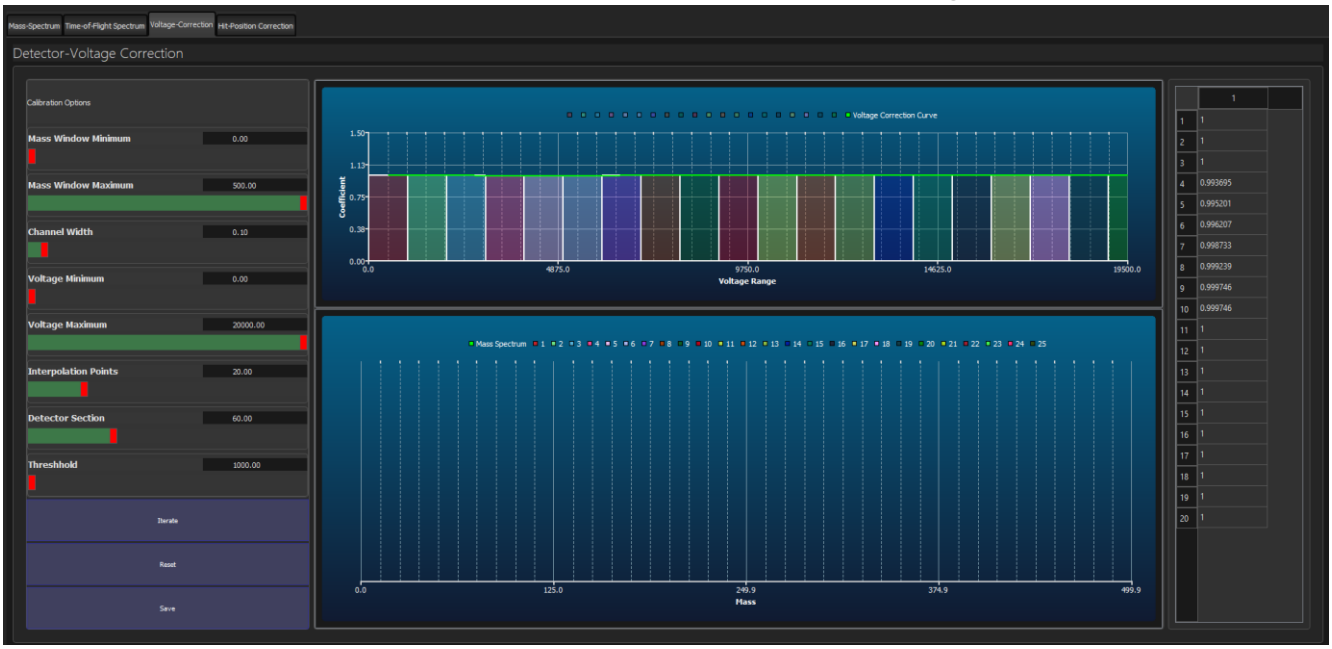
Once you are happy with a mass window you can click the Add Window button and the new mass window together with the element will be added in the alloy definition. You can do this process for all peaks displayed. To update the list of peaks you can press the Find Peaks button again. When closing this window you need to click the Refresh button in the Mass page to view the new windows.

Time-Of-Flight Spectrum

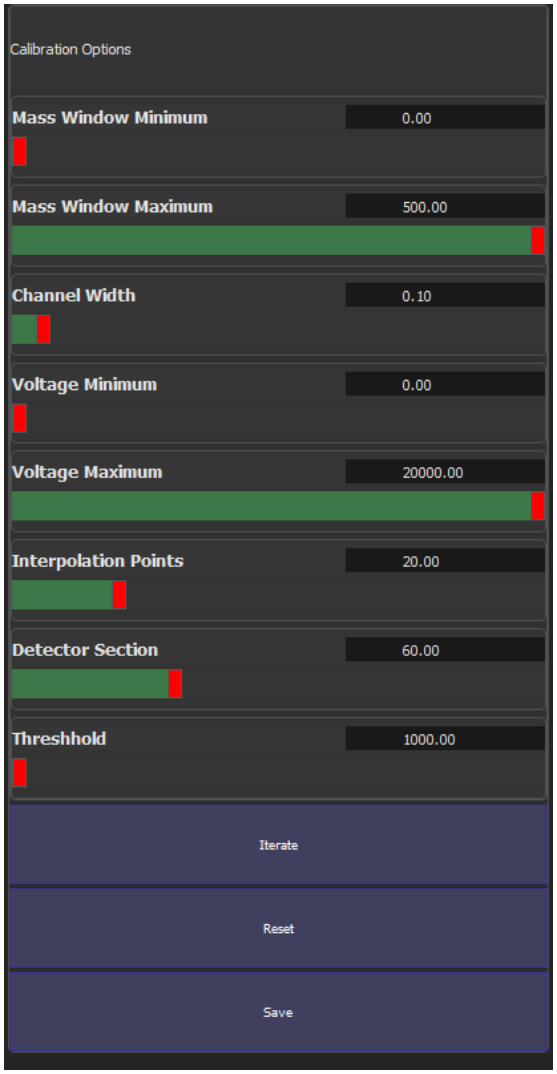
The Time-Of-Flight Spectrum is the second window on the Mass Tab. It displays a distribution of the Time-Of-Flights of all events.

Voltage Correction

The Voltage correction is the third window in the Mass Page. It allows the user to perform a correction on the masses based on the voltage of the events.



The window has 3 main parts. The left side contains parameters needed to calculate the correction and some buttons. The middle part contains 2 graphs, the correction windows and the factors on the top and the Mass Spectrum using the correction at the bottom. The right side contains a table of all the values that you can also modify manually.



The calibration options are as follows:

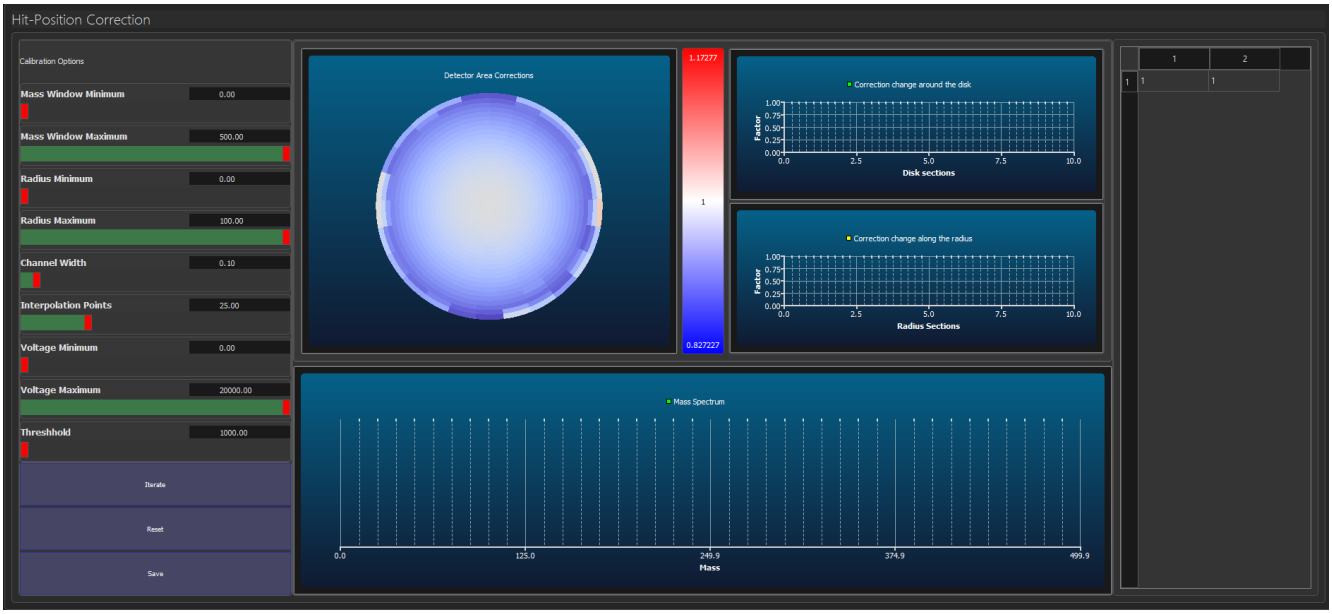
- Mass window Minimum and Maximum: you can set the minimum and maximum mass for which you want to calibrate
- Channel width: the width for every Mass Spectrum point. The lower it is the more precise is the mass spectrum
- Voltage Minimum and Maximum: The maximum and minimum values of voltage for which you want to calibrate
- Interpolation points: Specifies the number of voltage ranges to be created between the minimum and maximum voltage.
- Detector Section: specifies the radius of the detector for which you want to calibrate starting from the center of the detector.
- Threshold: The minimum number of events that a peak should contain for it to be considered.
- Iterate Button: performs one iteration of the voltage calibration. When finished the new factors are calculated and the Mass Spectrum corrected with the calculated factor is displayed. Several iterations may be needed to find the correct corrections
- Reset Button: resets all the correction factors to 1
- Save Button: Saves the current correction factors so that they can be applied to the Mass Spectrum. Use this when you are happy with the factors calculated.

The graphs react when an iteration is performed and update themselves.

The table of values also update automatically after every iteration and also allows for manual input of values.

Hit-Position Correction (HP Correction)

The HP correction assumes a circular Detector and divides it into smaller parts (pie slices and donut levels). Each of these parts (i.e. intersections of slices and levels) has a correction factor which is assigned to its center. Based on the position of every event a correction factor for its mass is calculated using bilinear interpolation of the 4 surrounding detector parts centers.



The circular chart is a color coded chart, using the color scale on its right, of all the factors. The two graphs on the right of the color scale react when you click a piece in the detector chart. The green chart display how the factors change along the disk (it is also painted in green in the detector chart. The first column of the left most table displays the exact values. The values start from 0 degrees (north part of the graph) and go all the way around clockwise. In the same way the yellow chart displays the factors along the radius. The second column also displays these values starting from the center of the detector.

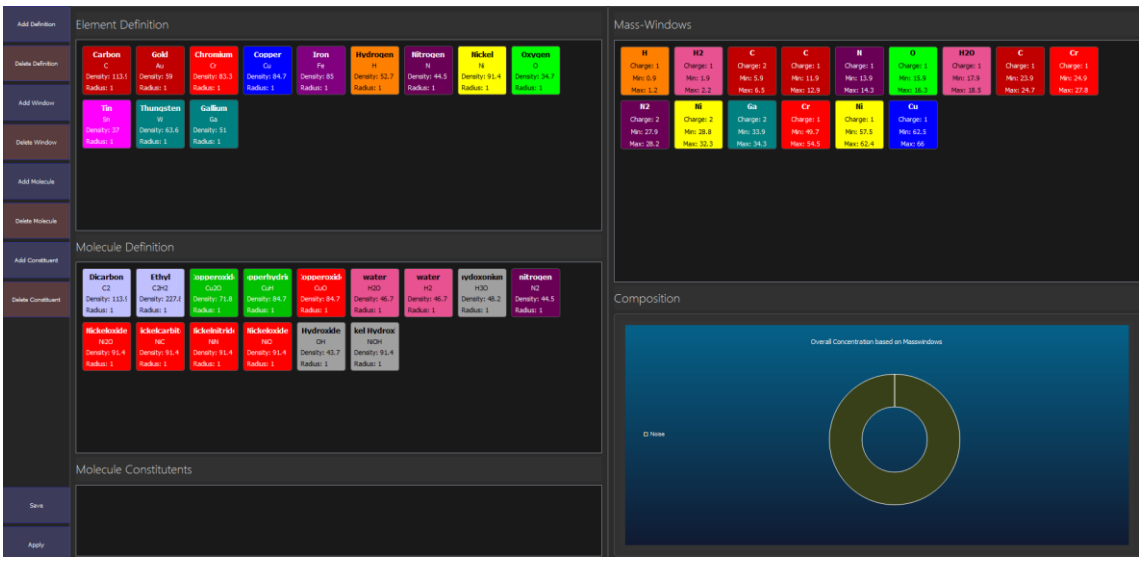
If you need to calculate them again then you will need to iterate several times to get the right values.

The controls on the left can help you with that. Mass Window, Radius and Voltage Min/Max filter the data that you want to use for this calibration. Channel width is the width of every mass bar. Interpolation Points is the number of disks and pie slices that are created. Threshold is the lower limit for a peak to be considered a peak.

When you click iterate, a mass spectrum is calculated using the current correction factors. The factor for every part of the detector is calculated so that the highest peak of events in that region si moved to the position of the highest peak in the center of the detector. Every time you iterate the new factors are used to calculate the mass spectrum. In order to save these factor for the current project you have to click the Save Button. The graph on the bottom of the screen shows the current Mass Spectrum after every iteration.

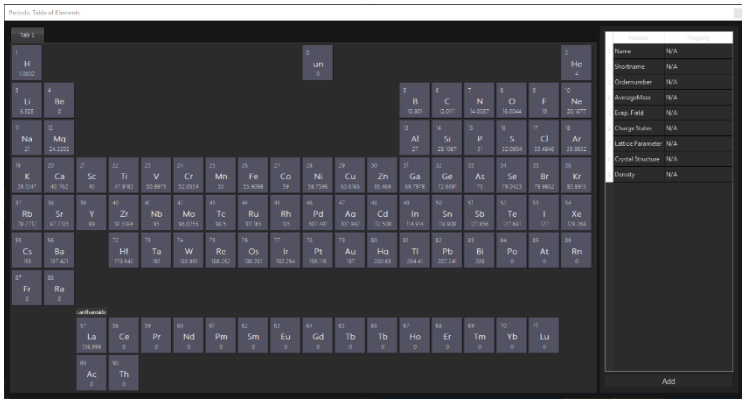
Alloy Tab

The Alloy Tab provides an interface to modify the Alloy definition of your project. If no definition is loaded then this page will be blank, but a new definition can be created from scratch. If a definition is loaded then you should see something like the image below.



Here you can manage your elements, molecules, molecule constituents and mass windows. To select one of the small cards you can right click on it. A white border will be drawn around the currently selected cards.

To create new definitions or delete existing ones you can use the buttons on the left side.



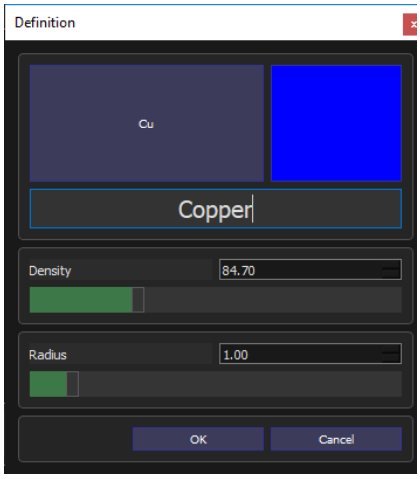
Add Definition opens up the periodic table and allows you to select an element and add it to the list of elements by clicking the add button. Clicking on an element will display the information of the element on the left side of the screen.

- Add Molecule will create a new molecule card that you can modify.
- Add Mass Window will create a blank Mass Window which you can modify as well. If you have already selected an element from the element cards that the mass window will be initialized with that element.
- Add constituent will add the currently selected element as a constituent to the currently selected molecule. If not molecule or not element is selected than a constituent will not be created.
- The Delete button will delete the currently selected card depending on which delete button you click.

Modifying a Card

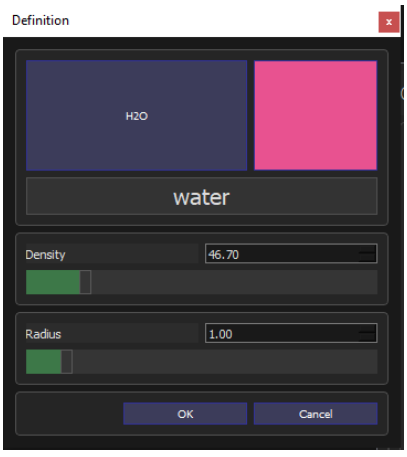
If you double click a card then a larger card will be shown where you can modify the information as follows:

- Element Definition



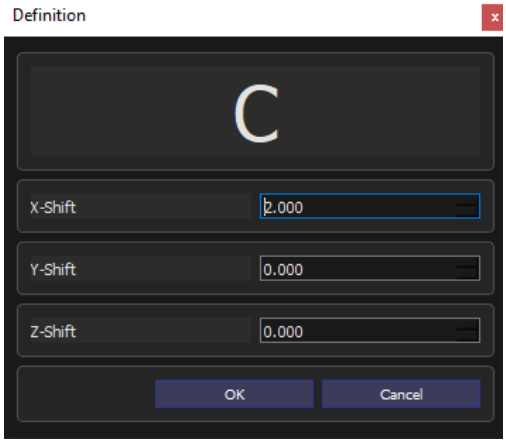
The large Button contains the symbol of the element. Clicking it allows you to change the element and choose new one from the periodic table.
Clicking on the color will allow you to modify the color of that element.
The name of an element can be modified as a text
Density and radius are 2 more parameters for the element that you can modify. Density should never be 0. To save the changes click OK.

- Molecule Definition



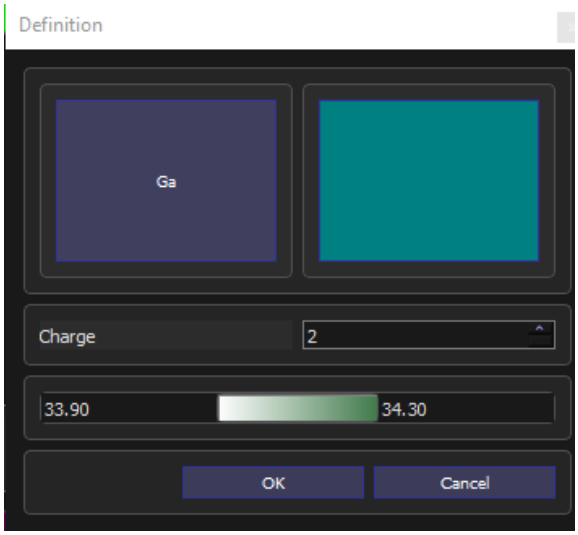
Works in the same way as the Element definitions. The only difference is that when you click the symbol button you have to manually input the symbol of that molecule

- Constituent Definition



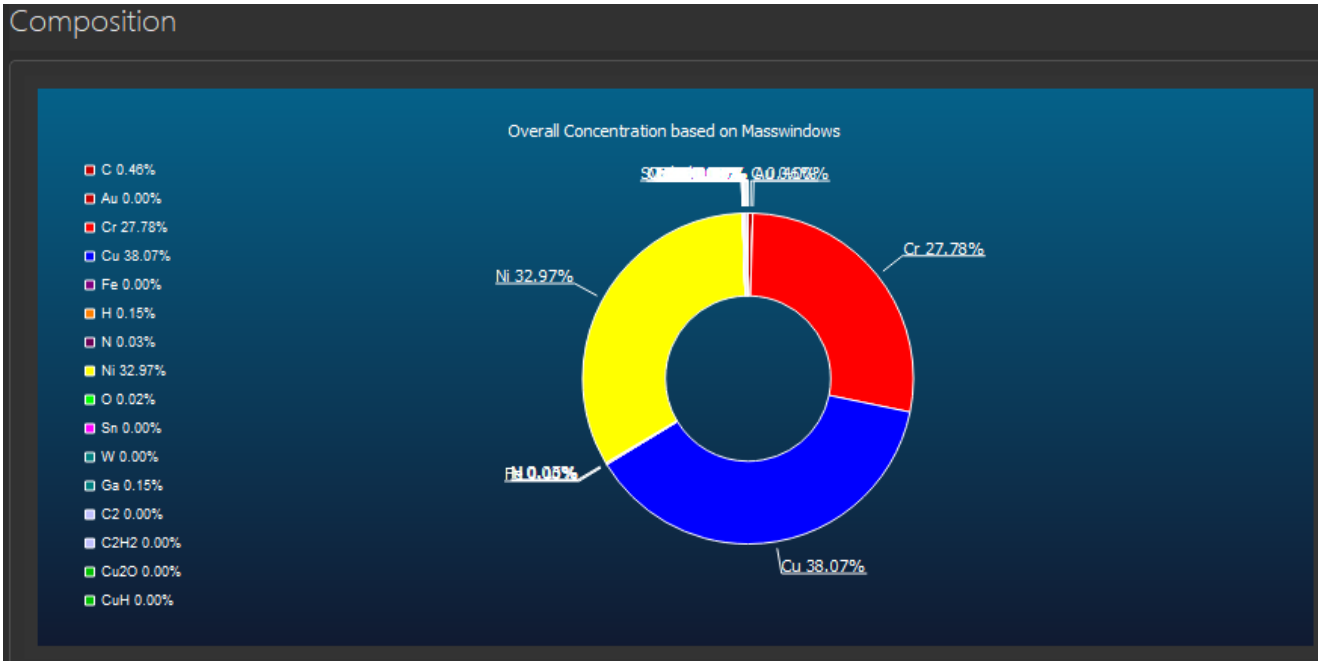
The constituent definition is very simple. The Symbol of the element specifies what element it is. The shift coordinates specify the position of that constituent with regards to the center of the molecule

- Mass Window definition



The mass window definition allows to change the element or molecule of that window. Zou can change that by clicking the symbol of the element/molecule. There you can select a new element/molecule from the list of the already defined ones.
The color is the same color of the element/molecule and cannot be changed from here but rather it is changed by modifying the element/molecule. The charge of the mass window can also be changed. The range at the bottom is the minimum and maximum mass that fall into it. Clicking Ok saves the changes.

The last 2 buttons in the left side are Save and Apply.
Save will update the alloy file(.aly) to contain the changes made to the definition so that you can load it at a later project.
The apply button will assign to every event an element based on which mass window their mass falls in. After applying the Composition chart will update to display the concentration of every element. Event that don't belong to any mass window are considered as noise.



The composition chart also displays what percentage of the non-noise data belongs to every element.

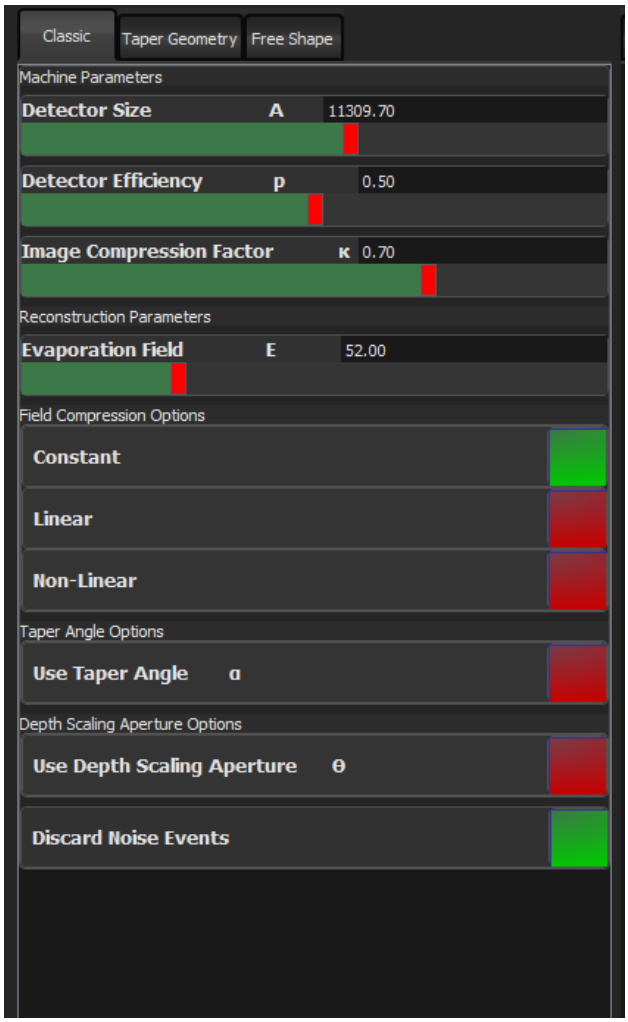
Reconstruction Tab

The Reconstruction Tab allows to calculate 3D coordinates of every event. Different Reconstruction modules are available. The Reconstruction Tab contains 2 charts:

a) Radius Evolution: where you can see how the radius evolves with depth.
b) Evaporation Field: where you can see how the evaporation field changes with depth

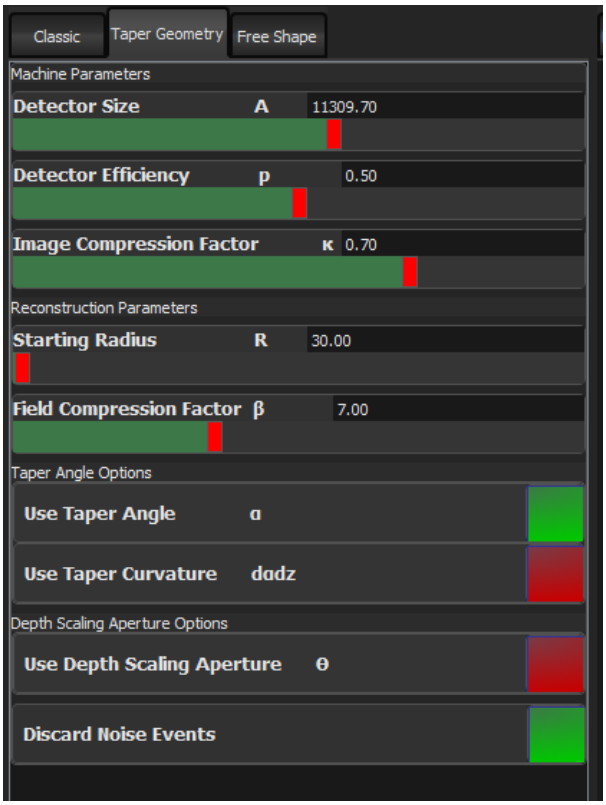
Both charts are filled with data once the Reconstruct button on the bottom-left side of the screen is clicked.
Each of the Reconstruction modules contains a number of parameters required to calculate the coordinates. These parameters are place on the left side of the screen.
The available modules are:

- Classic Module



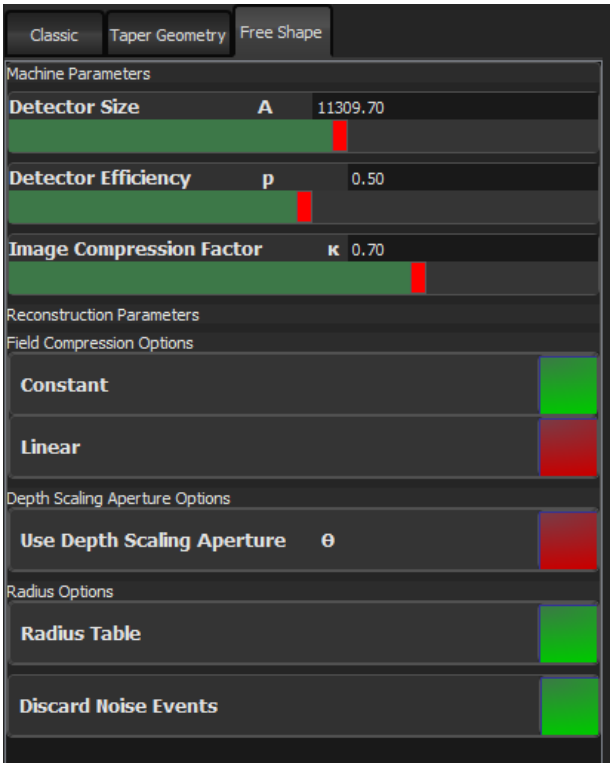
TODO – Description of Classic and all parameters

- Taper Geometry Module



TODO – Description of Taper Geometry and all parameters

- Free Shape Module

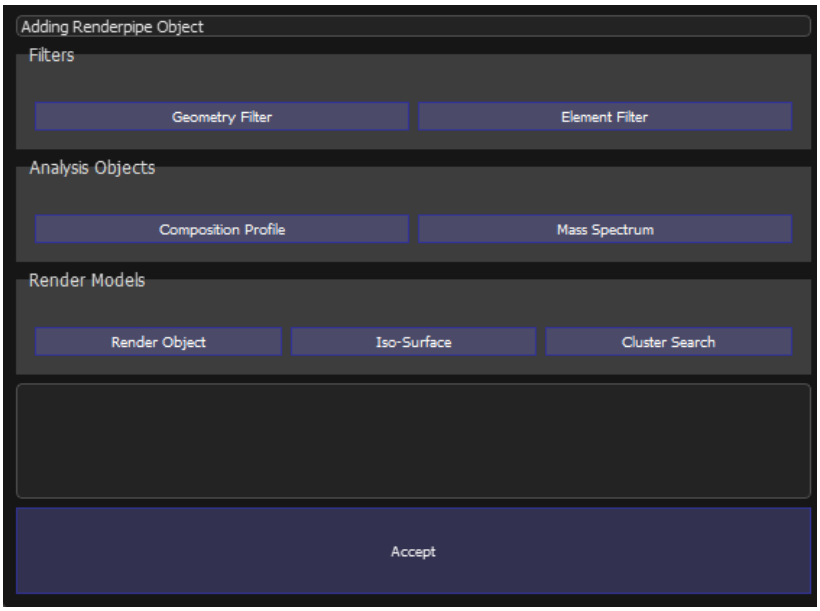


TODO – Description of Free Shape and all parameters

3D-View Tab

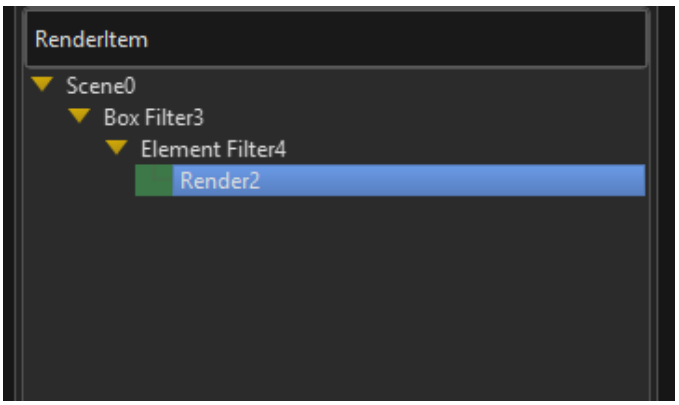
The 3D-View Tab provides a 3D canvas where you can view, manage and analyze your reconstruction. The left side contains a view with the main controls for the 3D-View. At first an empty 3D scene is created where you can add more objects.
On top of the view there are 2 buttons: Add and Delete.

Clicking the Add Button will open a new window where the user can decide what objects to add.



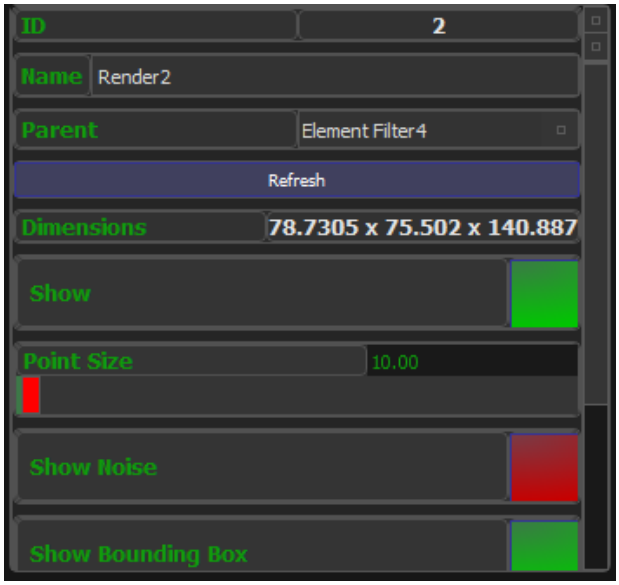
The available objects are divided in 3 categories:
- Filters: these objects filter out data. The filters are either geometry filters (cube, cylinder, sphere) and element filters. More on them later.
- Analysis objects: these analysis tools that can be added.
- Render Model: these objects create 3D structure that are rendered in the scene.

The Delete button allows you to delete an object you have created. All objects except for the Scene can be deleted.

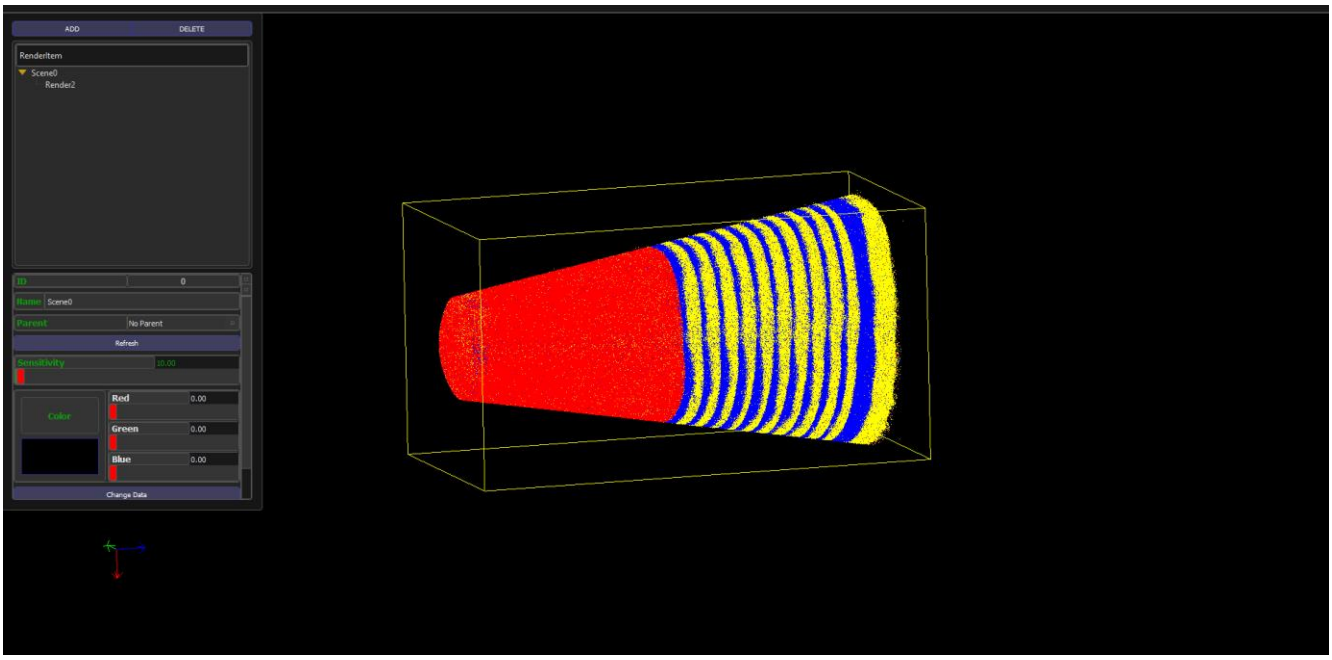


Below the Button there is the Render Tree. It contains a hierarchical structure of all the currently added objects. Data passes from the top level to all its children and from every child to its own children. In this picture the Scene passes the data to the box filter. The box filter out all elements and molecules that are on its outside

and then passes the data to the element filter. The element filter removes all elements and molecules of certain types (user decides) and then passes the data to the Render Object which displays every element and molecule in 3D.



At the bottom the properties of the currently selected object (blue background in the Render Tree) are displayed and allow the users to modify it to their needs. Each object has its own properties and when switching between objects the properties are updated.

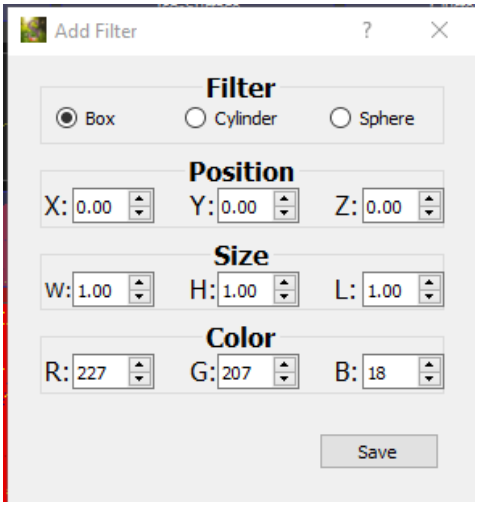


The rest of the page is the 3D Scene. Here all objects are rendered based on their properties and the hierarchies dictated by the Render Tree.

Render Tree Objects

It is possible to create the following objects in Scito from the Add Object interface:

GEOMETRY FILTER



When you select Geometry Filter a new dialog shows up where the type of filter (box, cylinder or sphere), position, size and color can be chosen. The position, size and color can also be changed later. Clicking save will create the desired object and show it in the scene. The Box, Cylinder and Sphere Filter are identical when it comes to properties and functionality. They receive the data from their parent and then remove all data that is outside and pass the remaining data to their children.

Properties

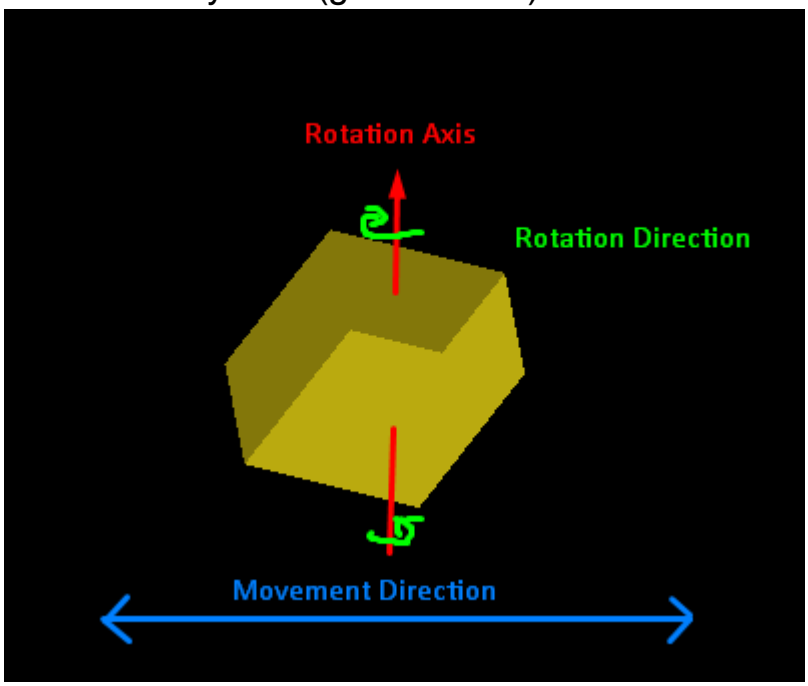
- ID: this is a unique number to identify the object. It cannot be changed.
- Name: the name of the object which is also what will be shown in the render tree. It can be modified so that it is something that the user can differentiate between objects
- Parent: This is the current parent of the object. The object will receive the data from its parent. To change it a new object can be selected from the dropdown list. The hierarchy in the render tree will change and the scene will be updated
- Width/Height and Depth: for the box this is the length from edge to edge in 3 directions. For the cylinder width and height are the diameters of the bases, while depth is the distance from base to base. For the sphere they denote the size of the radius in each of the 3 dimensions. Changing one of them while keeping the other 2 will deform the object (the cube can become a cuboid, the sphere can become an ellipsoid while the cylinder can become a cylinder with ellipse bases).
- Center X,Y and Z: these are the coordinates of the center of the object.

- Yaw, Pitch and Roll: These are the 3 angles that define the rotation of the object with regards to its own coordinate system.
- Transparency: 0 is a fully opaque object while 100 is a fully transparent object (i.e. cannot be seen in the scene)
- Selected: Red means the object is not selected while green means the object is selected. Only 1 filter object can be selected at any time. If an object is selected, then the mouse movements will affect that object. (more on this in the Controls section).
- Color: Changes the color of the object. You can enter the RGB values manually or click the color and then change it using the new dialog that appears.

Controls

A filter object can also be modified using mouse and keyboard input. To do so you have to first select a filter. You can do that by changing its Selected property to green or by holding SHIFT and left-clicking the desired object. When selected its color will become slightly brighter to show the fact that it is selected. To unselect an object either change its Selected property to red or hold SHIFT and left-click on the background of the scene.
Once a filter is selected several manipulations are available.
Scrolling up with the mouse wheel will increase its width, height and depth by the same value, making the object larger. Scrolling down with the mouse wheel will decrease its width, height and depth, making the object smaller. Holding X pressed while scrolling up/down will increase/decrease the width of the object. Holding Y pressed while scrolling up/down will increase/decrease the height of the object. Holding Z pressed while scrolling up/down will increase/decrease the depth of the object.
Holding the left mouse button while moving the mouse will move the object in the direction of the mouse movement. Holding Space pressed while holding the left mouse button and moving the mouse left or right will move the object back and forth in the screen (towards you or away from you).
Holding X pressed while holding the left mouse button and moving the mouse left or right will move the object in the x-direction of the coordinate system (red arrow). Holding Y pressed while holding the left mouse button and moving the mouse left or right will move the object in the y-direction of the coordinate system (green arrow). Holding Z pressed while holding the left mouse button

and moving the mouse left or right will move the object in the z-direction of the coordinate system (green arrow).



Holding the right mouse button and moving the mouse will rotate the object around a plane perpendicular to the direction of the mouse movement and parallel to the screen that passes through the center of the object like in the picture. This gives the use the ability to rotate in 2 directions. To rotate in the third direction (around an axis that is perpendicular to the screen plane and passes through the center of the object) you have to hold SPACE while doing the same as above.

Another way to rotate the objects is to hold X, Y, or Z pressed while holding the right mouse button pressed and moving the mouse left or right. This will rotate the object around its own x,y or z direction (axis that goes from the center of the object to the center of one of its face in the case of the cube)

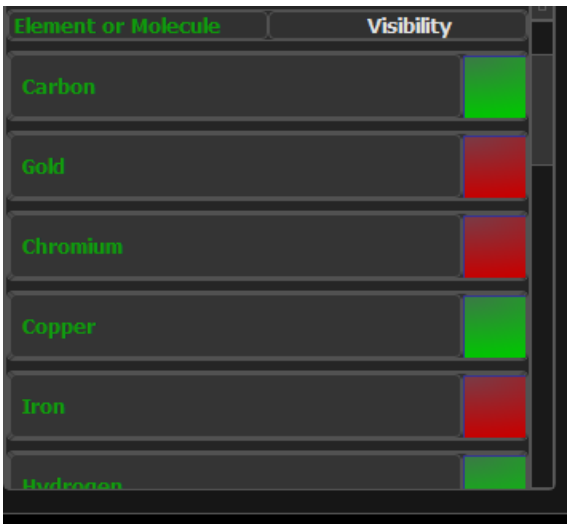
ELEMENT FILTER

An element filter can be used to filter out events based on the element/molecule that they are. The filtering occurs in real time so that the changes can be seen instantly.

Properties

- ID: this is a unique number to identify the object. It cannot be changed.
- Name: the name of the object which is also what will be shown in the render tree. It can be modified so that it is something that the user can differentiate between objects
- Parent: This is the current parent of the object. The object will receive the data from its parent. To change it a new object can be selected from the dropdown list. The hierarchy in the render tree will change and the scene will be updated

- A list of all elements and molecules with the visibility status: red means that that element is filtered out and will not be displayed while green means that that element is not filtered out and will be shown.



In this image Gold, Chromium and Iron are removed from the data that will be passed to the children, while Carbon, Copper and Hydrogen will be passed to the children. The status of every element can be modified at any time from the properties here.

COMPOSITION PROFILE

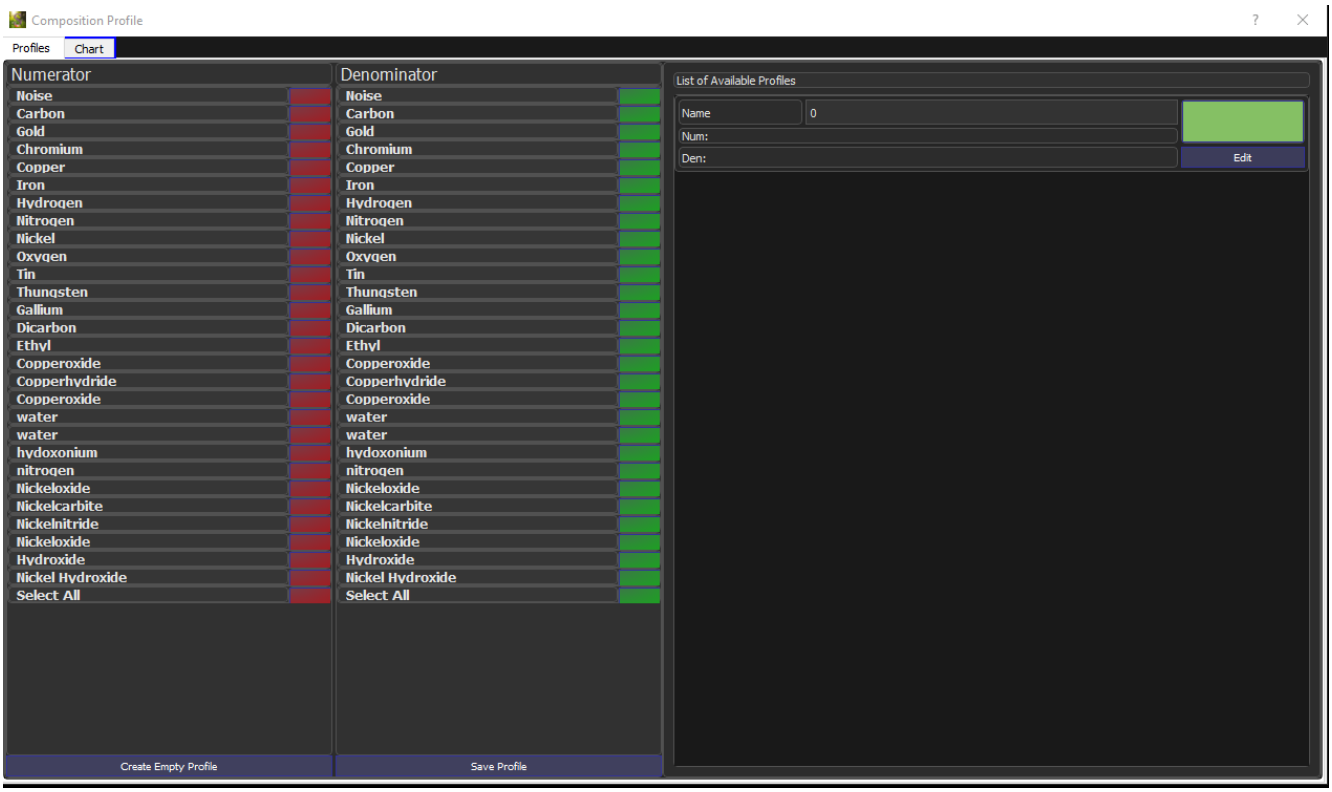
Composition Profile is an analysis tool that divides the data into slices along the z-direction. If a geometry filter is in the hierarchy of the composition profile (as a parent or parent of a parent) then the slices are created in the z-direction of the geometry filter. For example, if a cylinder filter is the parent of a composition profile then the slices are parallel to the bases of the cylinder.

Properties

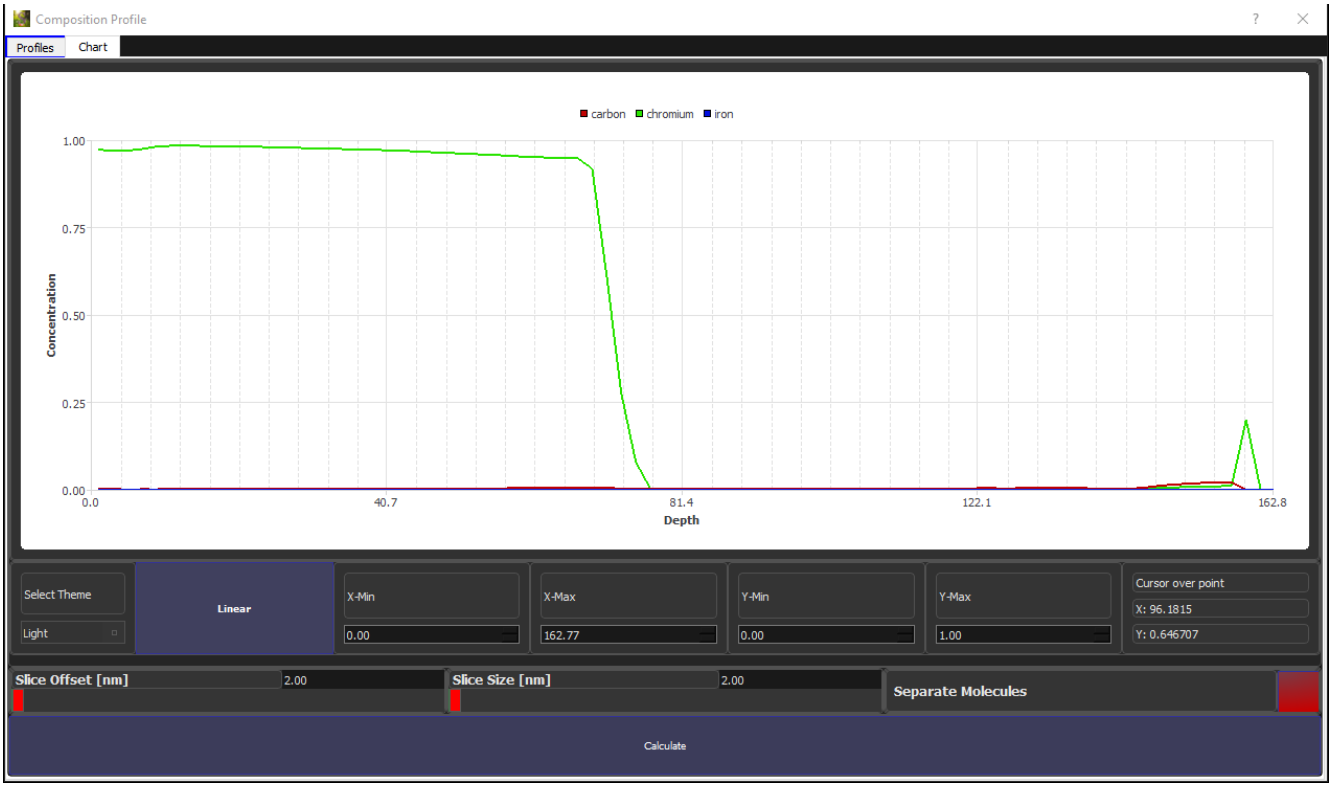
- ID: this is a unique number to identify the object. It cannot be changed.
- Name: the name of the object which is also what will be shown in the render tree. It can be modified so that it is something that the user can differentiate between objects
- Parent: This is the current parent of the object. The object will receive the data from its parent. To change it a new object can be selected from the dropdown list. The hierarchy in the render tree will change and the scene will be updated
- Auto-Refresh: when green the composition profile chart is updated automatically if changes happen to the data. It is advised to use it only when the amount of data is not high otherwise there can be lag in the update.
- Chart: pressing this button will open the Options of the Composition profile.

Composition Profile Options

The composition profile options window will open when you add a new composition profile. If you close it, you can re-open it by clicking the Chart button in the properties of the composition profile. In this window there are 2 tabs: Profiles and Chart.



The Profiles Tab allows you to create profiles. The list of profiles is displayed on the left side. Every profile contains a name which can be changed to any arbitrary text, a color which can also be change by clicking on it, a numerator list which contains all elements and molecules that are in the numerator of that profile, the denominator contains the list of denominator values and an Edit button that allows to make changes to the numerator and denominator. On the left side a list of all elements and molecules that can be selected for the numerator and denominator is displayed. The lists displayed are for the profile that is currently being edited. By clicking the edit button the list of that profile will be displayed and it will be possible to change that. In the list red means that that element is not added while green means that the element will be considered when counting the events. Clicking the Save Profile button will save the changes made to that profile. Clicking Create Empty Profile will add a new profile to the list and will open that profile for editing. For every profile it is necessary to click Save Profile at least once to save the changes.

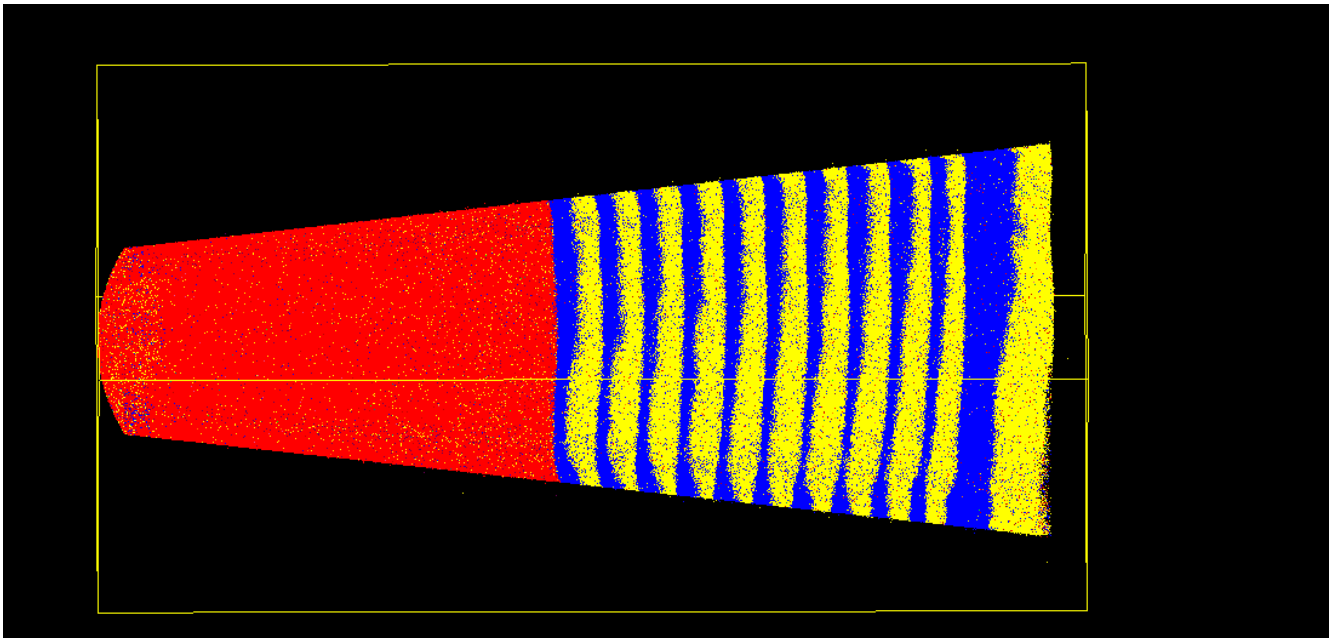


The Chart Tab contains a large chart where you can view the graph for every profile that you created. The x-axis is the depth of the slice while the y-axis is the concentration of the slice. If the denominator is 0 then the concentration of that slice is set to 0. Below the chart controls 3 parameters can be set. The slice offset is the distance between the starting points of 2 consecutive slices. The slice size is the length of a slice. If these 2 parameters are equal, then slice n+1 will start at the end of slice n. If Separate molecules is green, then every molecule is divided into its constituents. The constituents need to be defined in the alloy tab for this function to work correctly. Clicking Calculate will refresh the chart with the new values

MASS SPECTRUM

The Mass Spectrum object creates a mass chart using the data that it gets from its parent. This can be used to view a Mass Spectrum of only part of the data. Changes can be made to the mass windows and clicking apply will copy these changes to the alloy definition. In order to view your changes in the 3D scene then the reconstruction has to be reperformed

RENDER OBJECT



A render object is the 3D representation of the data where every element and molecule is displayed as a colored pixel.

Properties

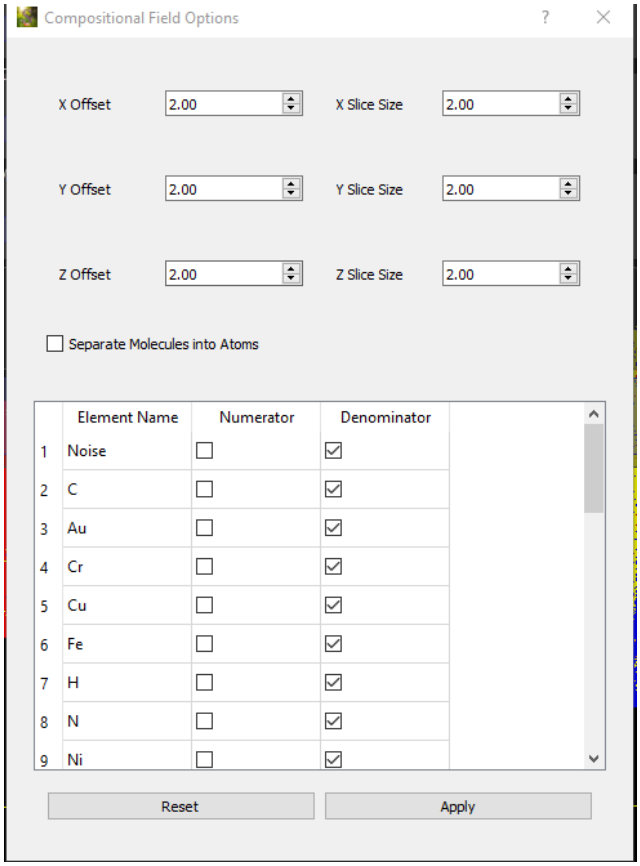
- ID: this is a unique number to identify the object. It cannot be changed.
- Name: the name of the object which is also what will be shown in the render tree. It can be modified so that it is something that the user can differentiate between objects
- Parent: This is the current parent of the object. The object will receive the data from its parent. To change it a new object can be selected from the dropdown list. The hierarchy in the render tree will change and the scene will be updated
- Dimensions: display the size of the whole 3D render objects (same as the dimensions of the bounding box.
- Point Size: increases the size of every point which makes them clearer when you zoom in.
- Show noise: if green it displays the noise events as black points in the 3D render. If red noise is not displayed but it it is not filtered out. The noise data is still there; it just is not visible.
- Show Bounding Box: if green shows a bounding box around the render object. If red, then the box is not shown.
- Bounding Box Color: Change the color of the bounding box.

Controls

The Render object cannot be moved, rotated nor scaled. In order to do that the camera has to perform these actions. How to do that is explained in the Scene object.

ISO-SURFACE

An isosurface is a 3d Object that renders a surface where the concentration of certain elements (selected by the user) is over a certain threshold (also chosen by the user). When first adding an iso-surface a menu appears where you can set the parameters of the iso-surface.



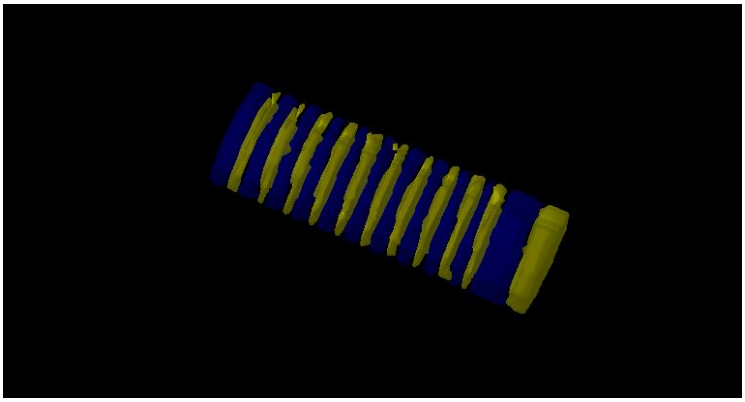
The offsets and slice size are analogous to those of the composition profile. The reconstruction is divided into cubes and the concentration of the elements in every cube is calculated. The data is then interpolated to find the correct position of the iso-surface. Again similar to the profiles in the composition profile, here you can choose which elements are in the numerator and which in the denominator. In the case of the iso-surface only 1 profile is allowed per object. To view 2 different iso-surfaces a new object has to be created.

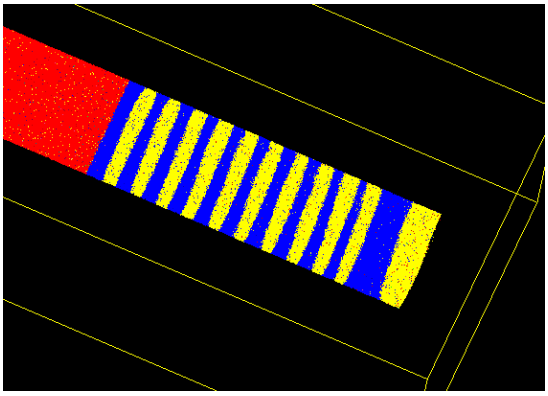
Properties

- ID: this is a unique number to identify the object. It cannot be changed.
- Name: the name of the object which is also what will be shown in the render tree. It can be modified so that it is something that the user can differentiate between objects
- Parent: This is the current parent of the object. The object will receive the data from its parent. To change it a new object can be selected from the

dropdown list. The hierarchy in the render tree will change and the scene will be updated

- Iso-Value: the concentration threshold in percentage.
- Transparency: 0 is a fully opaque object while 100 is a fully transparent object (i.e. cannot be seen in the scene)
- Iso-Color: color of the iso surface.





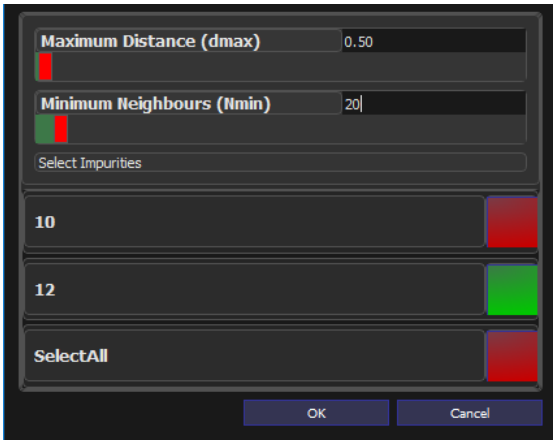
In the image on the left 2 iso surface objects are added. Each of them has an iso-value of 60% and they feature the concentration of 1 element over every other element. The image on the right displays part of the Render object. In both cases an invisible cylinder is filtering the data

Controls

The Render object cannot be moved, rotated nor scaled. In order to do that the camera has to perform these actions. How to do that is explained in the Scene object.

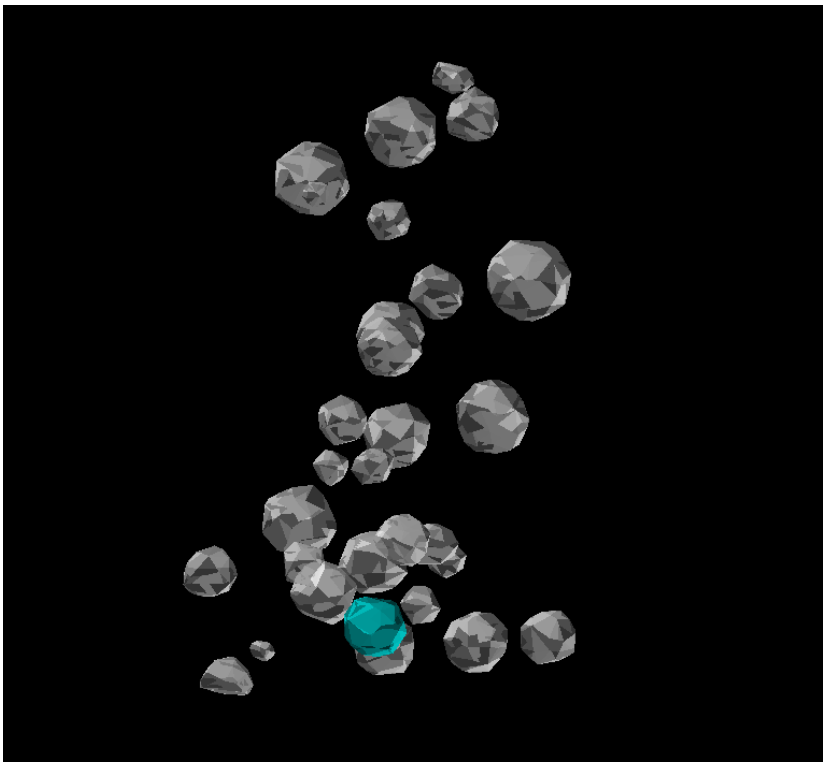
CLUSTER SEARCH

Cluster Search is another render model that displays the surface around a cluster of an element.



Adding a new cluster search will open this window where you can enter different parameters to find the clusters.
Maximum distance is the distance around an event where to look for neighboring points and Minimum Neighbors is the minimum number of neighbors an event should have in order to be part of a cluster. The events that will be considered for creating the clusters

are the impurities marked with green below that. After calculation the surface of the cluster will be rendered in 3d. The algorithm assumes that the clusters are convex. When first creating the cluster the color of one of them is different from the rest.



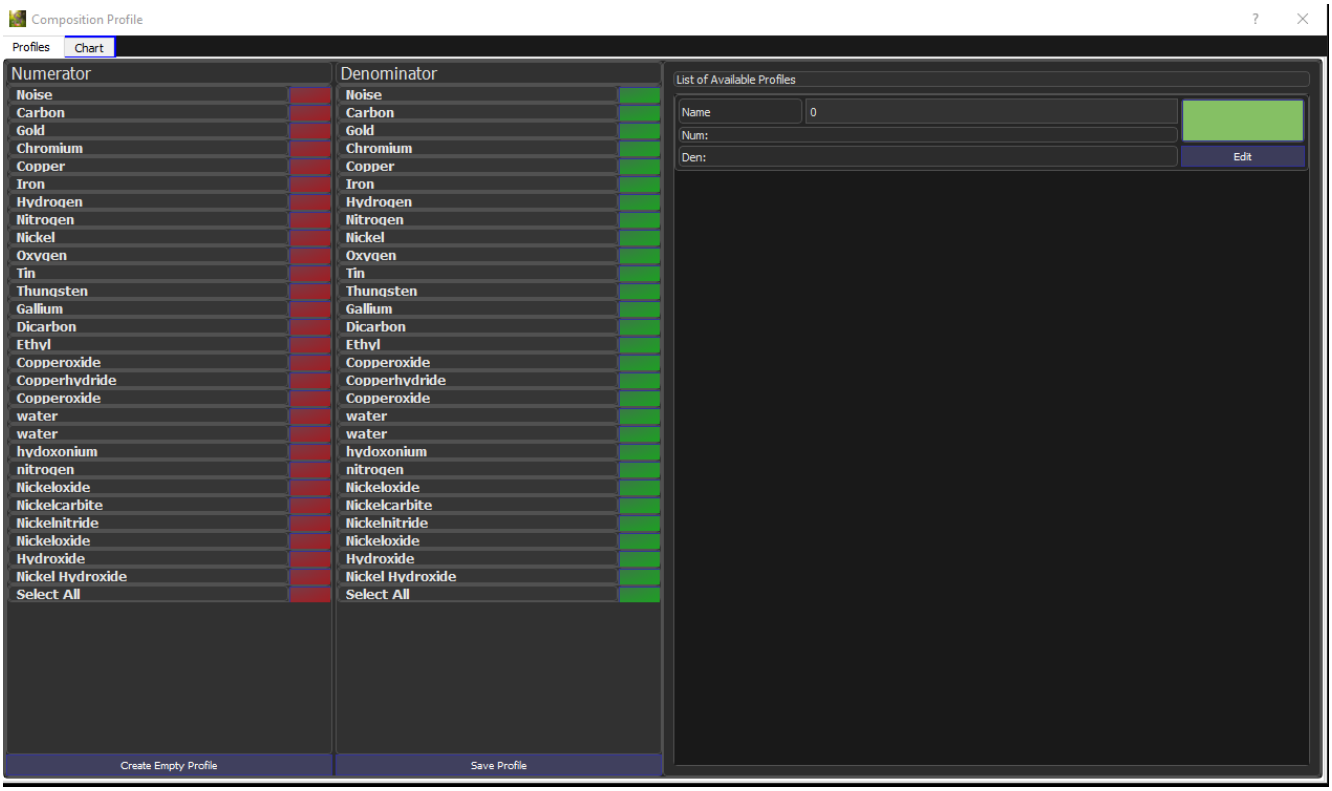
This is how a typical collection of clusters might look.

Properties

- ID: this is a unique number to identify the object. It cannot be changed.
- Name: the name of the object which is also what will be shown in the render tree. It can be modified so that it is something that the user can differentiate between objects
- Parent: This is the current parent of the object. The object will receive the data from its parent. To change it a new object can be selected from the dropdown list. The hierarchy in the render tree will change and the scene will be updated
- Color: Color of the cluster
- Transparency: 0 is a fully opaque object while 100 is a fully transparent object (i.e. cannot be seen in the scene)
- Proxygram: when clicking this button, the proxygram window will show.

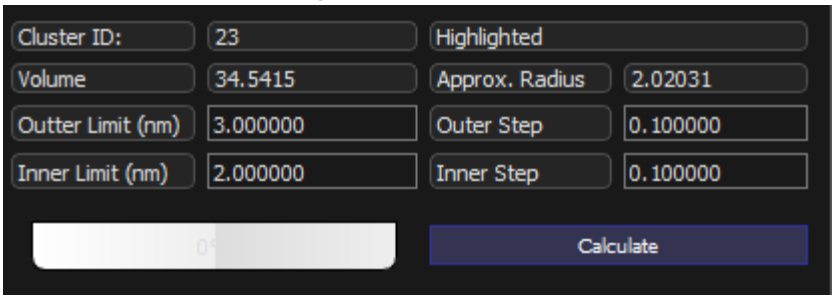
Proxygram

The proxygram window can be open by clicking the proxygrm button in the properties of the cluster search object. In this window there are 2 tabs: Profiles and Proxygram.

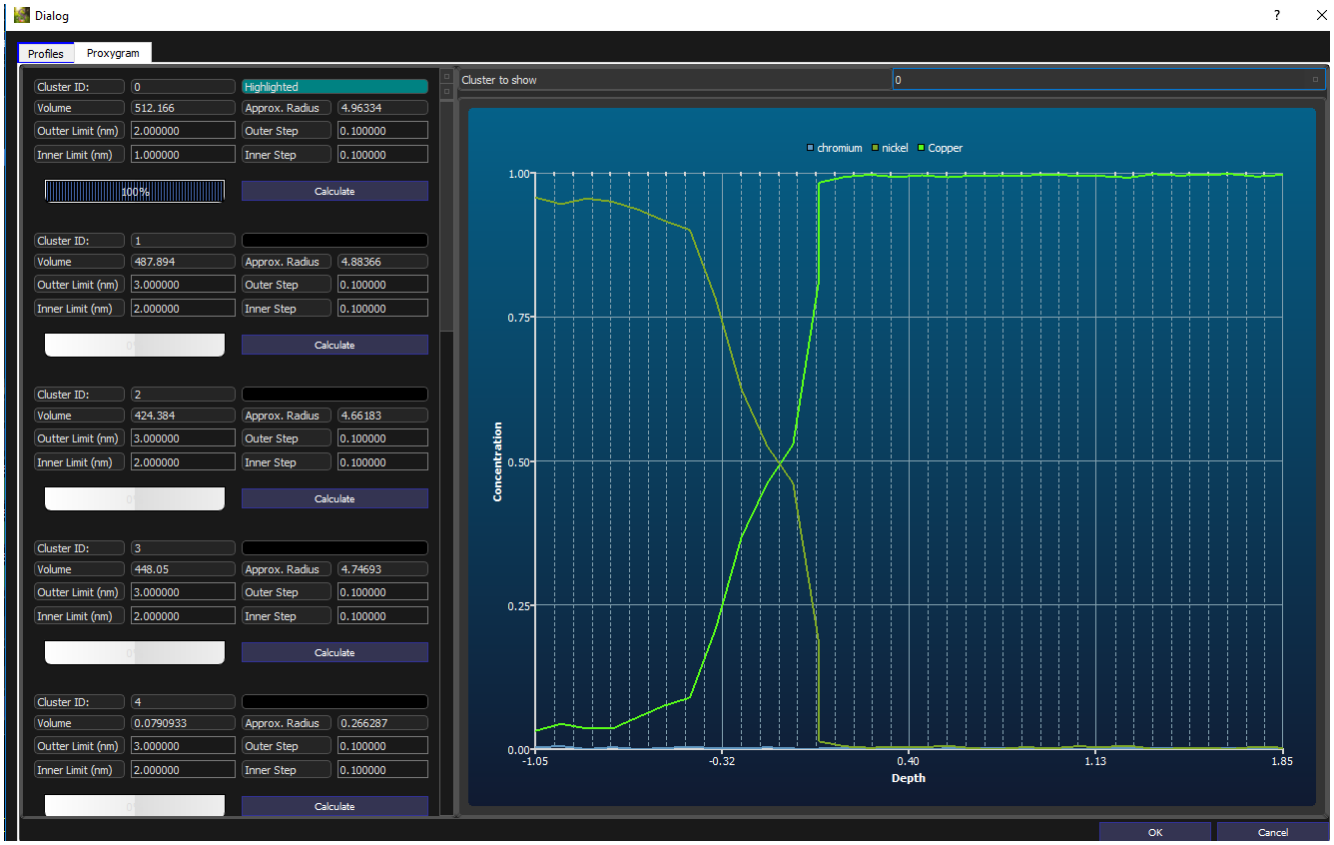


The Profiles Tab allows you to create profiles. The list of profiles is displayed on the left side. Every profile contains a name which can be changed to any arbitrary text, a color which can also be change by clicking on it, a numerator list which contains all elements and molecules that are in the numerator of that profile, the denominator contains the list of denominator values and an Edit button that allows to make changes to the numerator and denominator. On the left side a list of all elements and molecules that can be selected for the numerator and denominator is displayed. The lists displayed are for the profile that is currently being edited. By clicking the edit button the list of that profile will be displayed and it will be possible to change that. In the list red means that that element is not added while green means that the element will be considered when counting the events. Clicking the Save Profile button will save the changes made to that profile. Clicking Create Empty Profile will add a new profile to the list and will open that profile for editing. For every profile it is necessary to click Save Profile at least once to save the changes.

The proxygram window contains a lot of information.
On the left side a list of all the clusters and their options is displayed. For each cluster the following options are available:



- Cluster id: id for the cluster to differentiate between them. The cluster id increases in the z-direction.
- Highlighted is displayed if this cluster is the one with the different color in the 3d view. You can change the highlighted cluster in the 3d view. To change the selected cluster, you have to select the cluster search object in the Render tree and use the Up and Down keys in your keyboard. The currently selected cluster will have a different color compared to the other clusters
- Volume is the volume in nm3 of the current cluster.
- Approx Radius is the radius of a sphere with the above volume. (Note: clusters are not spheres, but this value can help determine the next values)
- Outter and inner limits (in nm): here you can enter a value of how much you want to go outside and inside the cluster to create the proxygram.
- Outter and inner step is the step that you want to use to create slices outside and inside the cluster. The number of slices is limit divided by step.
- Calculate will calculate the concentration of the profiles in every slice. You can calculate several proxygrams at the same time with the calculate buttons and their current progress will be displayed on the left of the calculate button. Once calculation is done you can change the cluster to show property on top of the graph and select one of the cluster ids that you have calculated to view it in the graph. If it has not been calculated yet, then an empty chart will be shown. Otherwise a chart like this should be shown.



SCENE OBJECT

The scene object is the main object of the 3D-View. It contains a canvas where all other objects are rendered. Also it allows for interactions and contains the data that is passed to all other objects.

Properties

- ID: this is a unique number to identify the object. It cannot be changed.
- Name: the name of the object which is also what will be shown in the render tree. It can be modified so that it is something that the user can differentiate between objects
- Parent: This is the current parent of the object. The object will receive the data from its parent. To change it a new object can be selected from the dropdown list. The hierarchy in the render tree will change and the scene will be updated

- Sensitivity: the overall sensitivity of the mouse movements. Increasing it will make movements faster while decreasing it will make them finer.
- Color: the color of the background
- Change Data: Clicking on this button opens a window where an .xyz file can be chosen and loaded. The current data is removed and replaced by the data in the .xyz file. When loading such a file the functionality of the 3D-View will still be available while the functionality of the other tabs will not be possible anymore as the required information is not exisiting.
- Rounded Points: by default, every atom/molecule is displayed as a pixel. If rounded points is green, then the events will be displayed as rounded objects giving a better representation. Combining this property with a large Point size in the Render object can create realistic more realistic images.

Controls

The scene object also contains a camera that can be manipulated. In order to do so no all geometry filter objects need to have the selected property red. The following movements are possible with camera.
Pressing R will reset the camera to its initial position
Pressing SHIFT + X, Y or Z will orient the camera so that the x-axis, y-axis, z-axis respectively of the coordinate system points towards you.
Pressing CTRL + X, Y or Z will orient the camera so that the x-axis, y-axis, z-axis respectively of the coordinate system points away from you.
Scrolling the mouse wheel out will zoom in the scene.
Scrolling the mouse wheel in will zoom out the scene.
Holding the left mouse button while moving the mouse will move the camera so that it looks that the objects move in the direction of the mouse
Holding X, Y or Z pressed while holding the left mouse button pressed and moving the mouse left or right will move the camera in a direction so that it looks that the objects move in the x, y or z axis respectively.
Holding the right mouse button clicked while moving the mouse will rotate the camera around so that it looks that the objects rotate around an axis perpendicular to the mouse movement and that passes through the center of the Render object.
Holding SPACE while holding the right mouse button clicked while moving the mouse will rotate the camera around so that it looks that the objects rotate around an axis perpendicular to the screen plane and that passes through the center of the Render object.

Holding X, Y or Z pressed while holding the right mouse button clicked while moving the mouse will rotate the camera around so that it looks that the objects rotate around an axis parallel to the x, y or z axis of the coordinate system that passes through the center of the Render object. This is the same rotation as before but it eliminates small movements of the mouse in an undesired direction.
Pressing P will open a window where the current 3D scene can be saved as a picture.

FILES

Scito allows for its data to be exported into different files. That can be done using the Export functionality in the project Tab. The available file formats are as follows:

- Raw file (.raw): this is the most important file type. In order to start working with Scito you need such a file. It contains all the information for every event detected. If the raw data is filtered (using the filters in the raw-data tab) the remaining information can be save in a new raw file.
- Parameter file (.par): this file contains relevant machine parameters used by Scito. This file is not required to work with Scito as its information can be manually entered using the UI but since the machine parameters don't change from measurement to measurement having such a file can save a lot of time.
- Alloy file (.aly): this file contains the alloy definition of a project. Again it is not required to have this file as the definition can be create in Scito, but sometimes it can be useful to have one.
- Settings file (.set): this file contains parameters used in Scito that are not part of the parameter file. They can vary from measurement to measurement. Saving a project will automatically create this file.
- RTI file (.rti): This file contains the hierarchical structure and important properties of every object in the render tree of the 3D-View. Saving a project will automatically create this file.
- POS file (.pos) This file contains binary float data in the following order: reconstructed x, y, z positions (nm), mass (amu) using 32 bit big-endian.
- EPOS file (.epos): This file contains binary float data in the following order: reconstructed x, y, z positions (nm), mass (amu), time-of-flight (ns), standing voltage (V), pulsed voltage (V), ion impact x and y position (mm), pulse number since last ion impact, hit multiplicity. First nine values are floats followed by two unsigned integers using 32 bit big-endian.
- ATM file (.atm): This file contains an Ascii header and binary float data in the following order: reconstructed x, y, z positions (nm), atomID, mass (amu) using 32 bit little-endian.
- Composition profile file (.csp): this is an Ascii file that contains information on a composition profile.
- Composition field file (.csf): this is an Ascii file that contains information on an iso-surface.

- XYZ file (.xyz): this is an Ascii file with a header and the information such as atomID, reconstructed x,y,z position (nm) and mass (amu).
- Normalized XYZ file (.xyzn): This is the same as the XYZ file with the difference that the reconstructed positions are normalized to a coordinate system of a geometry filter so that the edges of that filter are the -1 and 1 values. This way all values will be between -1 and 1.

HIDDEN CONTROLS

In Scito there are also hidden controls that were not mentioned in this manual.

CHARTS

To activate the hidden controls on a chart, it first needs to have focus (by clicking it once). Every chart can be manipulated using these controls:
LEFT and RIGHT buttons will move the right border of the chart.
Holding SHIFT while pressing LEFT and RIGHT buttons will move the left border of the chart.
UP and DOWN buttons will move the upper border of the chart.
Holding SHIFT while pressing UP and DOWN buttons will move the lower border of the chart.
Double-Clicking on a chart will open a dialog that can create a text file with all the coordinates of every series in that chart.