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Hurricane

# Hurricane User's Manual

**Version 1.5**

**SAMx**

SAMx - Hurricane Hurricane User's Manual, Version 1.5

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# Introduction

Hurricane is an off-line computation program which deals with electron interaction. This program is therefore a new player in the Monte Carlo category.

Hurricane is based on the developments done in the last 20 years by Jean Henoc, Françoise Maurice, Jean-Louis Pouchou and Françoise Pichoir.

Hurricane is not quite similar to existing Monte Carlo programs and has some specificities:

- Full computation of individual interactions (Diffusion, lost energy, production of photons and electrons).
- Take into account secondary electrons and phenomena induced by the faster electrons.
- Computation done from the theoretical laws, no average formulas and no adjustments.

Hurricane main goal is to try to help when regular analytical quantitative methods are not valid.

- Heterogeneous chemical samples.
- Rough samples
- Particles in a different matrix.
- Specific geometries

To achieve this goal, Hurricane is based on a networking of the space, allowing it to be divided in very small pieces in which events can be studied. At the same time, complex geometries can be defined by combining primitives (spheres, cylinders, rhomboedra). This allows any sample to be described : precipitates of any form and any chemistry defined within a matrix.

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# Starting Hurricane

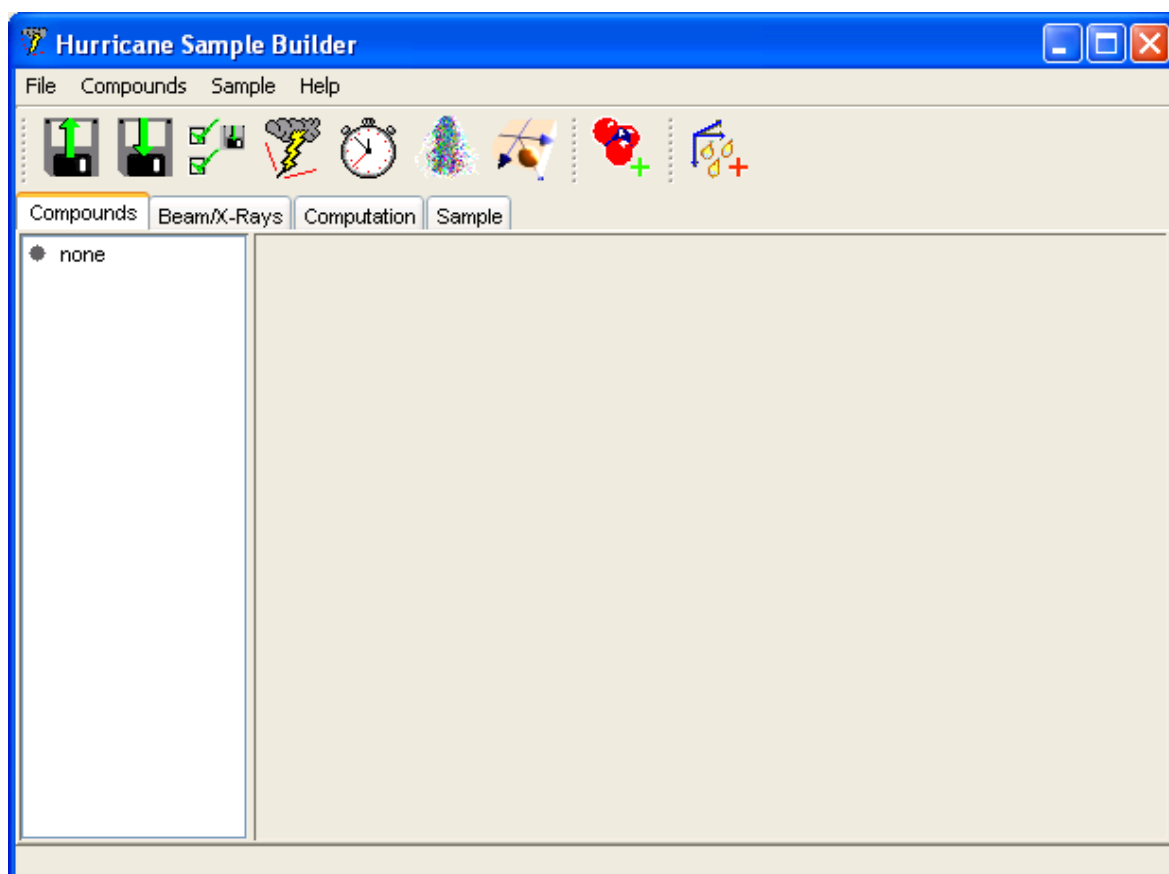
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## Launch the application



Launch the application by double clicking on the specific icon.

After a few seconds the main window is opened as shown below:



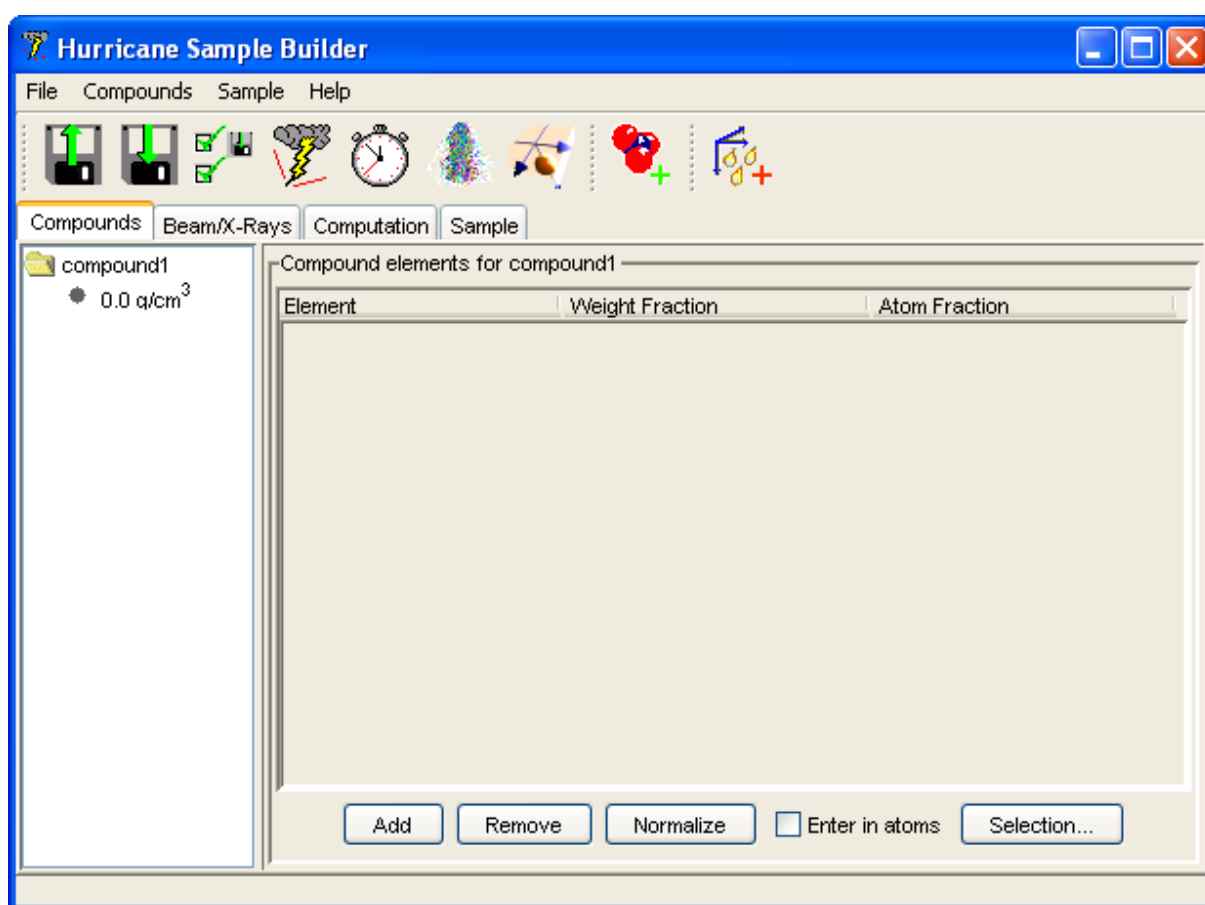
# Chemical sample structure / Compound

## Add a compound

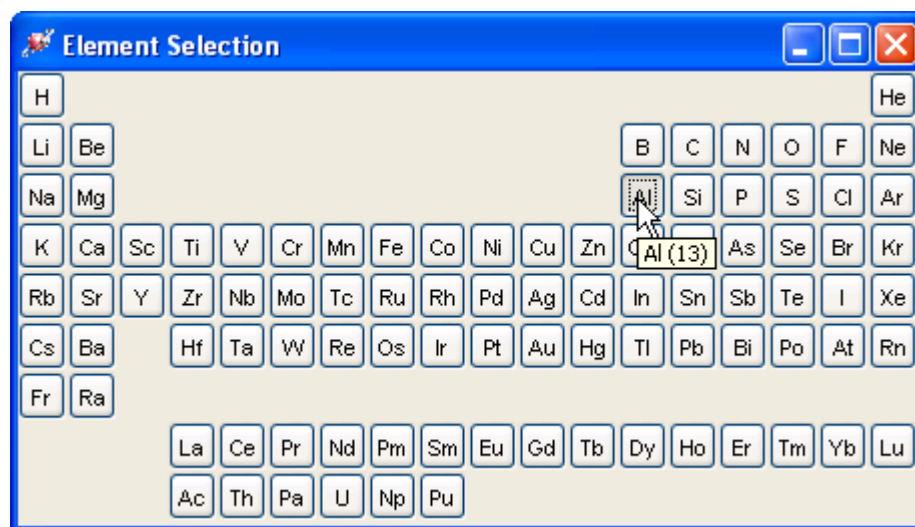
To add a compound, either click on the corresponding Compound button or go through the Compound menu:



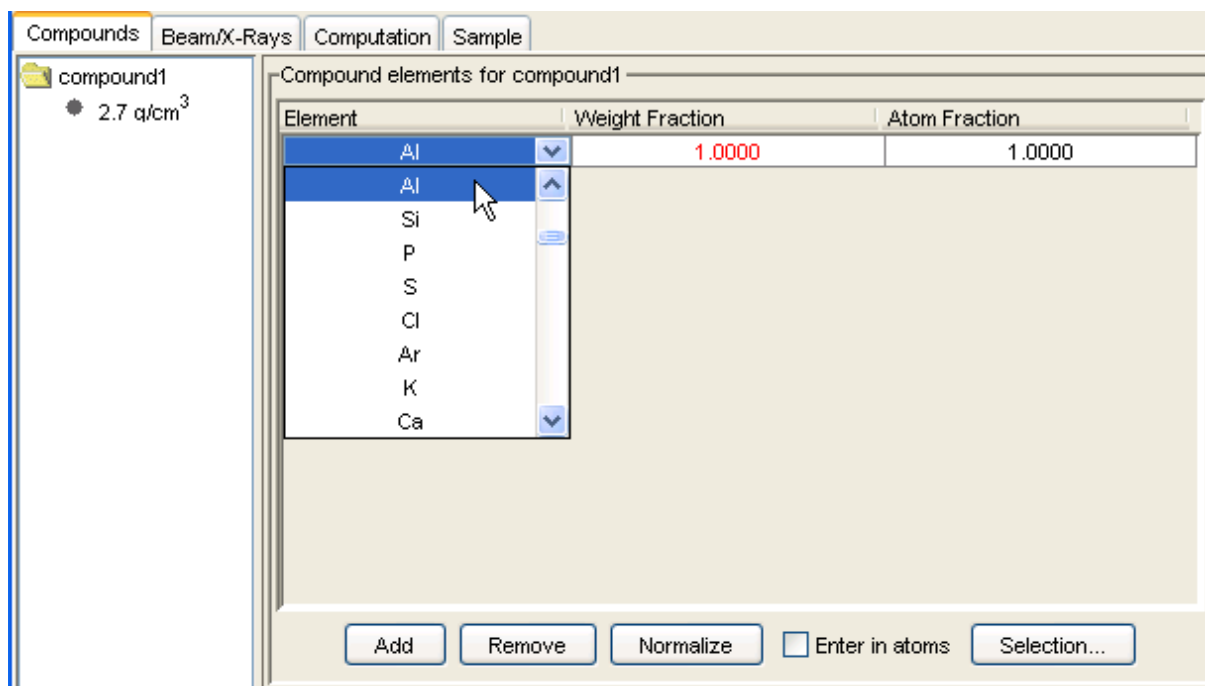
The window is then updated:



To add or delete an element, click on the Selection... button, then click once with the mouse left button on the corresponding cell in the popup window to select or deselect the element.

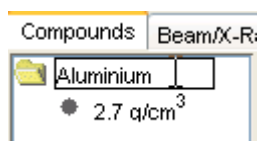


Another way to add an element, click first on the Add button, then select the elements in the element list, you can either go through the list or type the first character of the element name you wish to select. You can obviously add several elements, and then you need to define the composition using either weight or atom fraction. Do not forget to normalize fractions by clicking on Normalize.

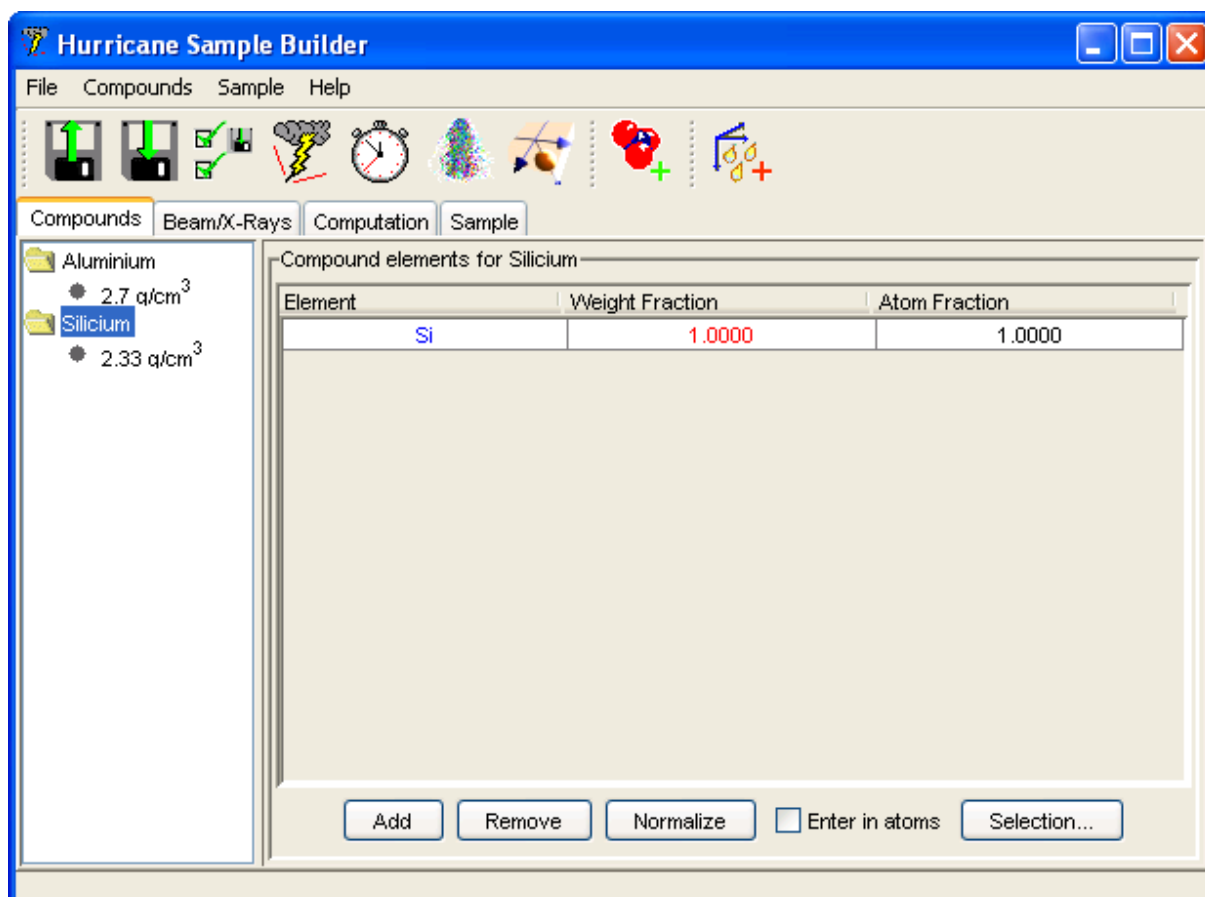




The name of the compound is automatically generated ( compoundX by default). The name can be changed by single clicking on the name itself, once the new name is entered, enter return.



The same method is used to define another compound, in our example, there is only one element (Si), the window should look like the one below.



# Experimental conditions

## The Beam/X-Rays Tab

Click on the Beam/X-Rays Tab, the user interface should then be as below:

The screenshot shows the Hurricane Sample Builder application window with the Beam/X-Rays tab selected. The interface includes a menu bar (File, Compounds, Sample, Help), a toolbar with various icons, and several configuration panels. The Accelerating Voltage is set to 15.0 keV, and the Energy Range is set to 16 eV - 30 keV. The Mode is set to Spot. The Center panel shows X Origin (nm) and Y Origin (nm) both set to 0. The Density panel shows Uniform selected and Gaussian unselected, with a Diameter of 1 nm. The X-Ray Lines Selection table lists elements Al and Si, both with X-Ray Lines set to K and a Variance Reduction Factor of 1.

| Element | X-Ray Lines | Variance Reduction Factor |
|---------|-------------|---------------------------|
| Al      | K           | 1                         |
| Si      | K           | 1                         |

To select the X-ray line, click on the already defined X-ray line.

This screenshot shows the same Hurricane Sample Builder interface, but with a dropdown menu open for the X-Ray Lines column in the X-Ray Lines Selection table. The dropdown menu shows three options: K, K, and L. The first two options are highlighted in blue, indicating they are the currently selected lines for the elements Al and Si respectively.

| Element | X-Ray Lines | Variance Reduction Factor |
|---------|-------------|---------------------------|
| Al      | K           | 1                         |
| Si      | K           | 1                         |

You should be aware that the possible X-ray line depends on the acceleration voltage entered in the same window.

Since Hurricane 1.5, the energy range can be customized, however in most cases, the default should be enough, provided that the acceleration voltage is not higher than the maximum of the energy range. See the special section on how to customize the energy range if you require it.

| Element | X-Ray Lines | Variance Reduction Factor |
|---------|-------------|---------------------------|
| Al      | K           | 1                         |
| Si      | K           | 1                         |

Enter the origin of the beam, the default values are (0,0) which correspond to the center of the sample. In this version only a uniform density of the beam is available, the diameter in nm can be entered in the corresponding field.

# Definition of the geometry

---

## The simulation algorithm

The simulation algorithm requires a division of the sample in a three dimensional grid of cubes. The choice of the dimension of the cubes is based on two contradictory principles.

First the computation box should be big enough, compare to the unit cell, otherwise the electronic trajectories will be stopped because of an intersection with the border of the analytical area. This will lead to a miss-estimation of the backscattered electron and other electron production. The computation box also depends on the accelerating voltage, higher kV implies a higher diffusion volume. The same volume will also depend on the element analyzed and specifically to the density considered.

Last if one wish to study more or less fine profiles of results, the unit cell should be of a comparatively thin size. Fortunately, sample geometry finer details are not restricted anymore to boxes of the unit cell size, as it was in Hurricane 1.0. Anyway, one should remember that the unit cell should not be too big, or this will increase the required CPU RAM to run the simulation. Typically one should not go over a 120x120x120 grid of unit cells.

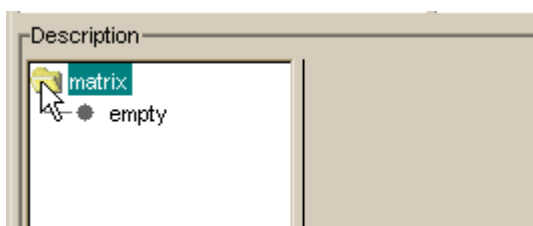
Practically, this last limitation needs to be kept in mind, remember that the adjustment of the overall box size can be done immediately after the simulation beginning as it will be seen later.

Click on the Sample tab, and define the computation box XxYxZ as 1000x1000x500 and the unit cell as 10x10x10.

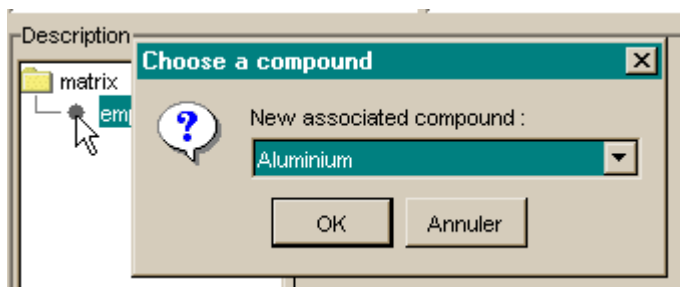
| Computation Box     | Unit Cell         |
|---------------------|-------------------|
| Size in X (nm) 1000 | Unit in X (nm) 10 |
| Size in Y (nm) 1000 | Unit in Y (nm) 10 |
| Size in Z (nm) 500  | Unit in Z (nm) 10 |

The Z axis is oriented in the depth direction, the Z zero corresponds to the surface of the sample. X=0, Y=0, correspond to the center of the sample.

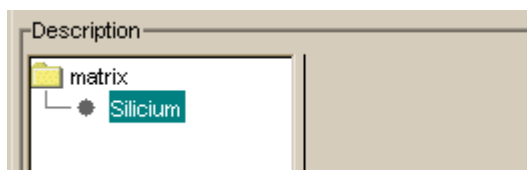
Once the computation box has been chosen, one needs to define the different compounds in the sample. To define a Silicon substrate simply double click on the matrix topic.



Now double click on the empty topic to open a new window.



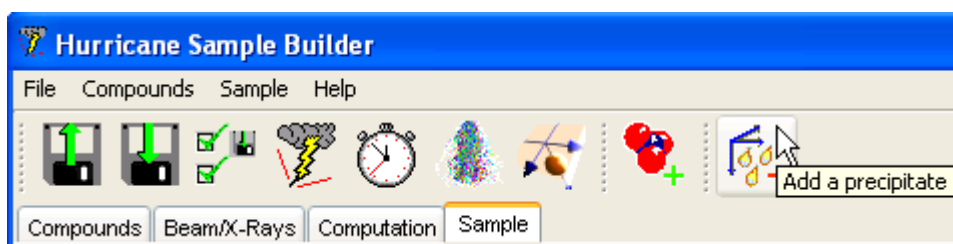
Select in the list the compound associated with the matrix to replace the default empty topic.



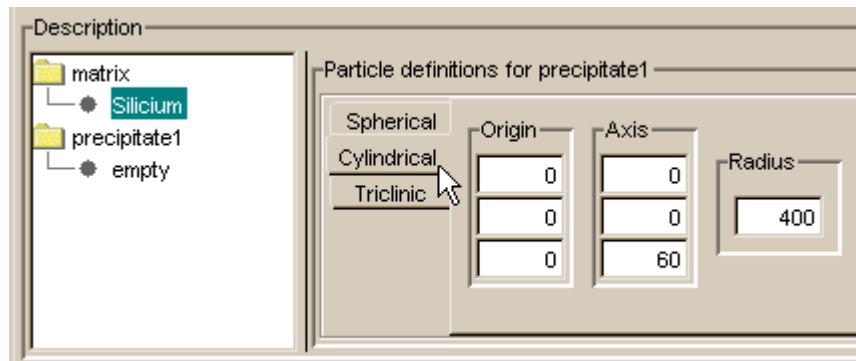
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## Adding a cylinder

Click on the precipitate button to add on top of the Silicon substrate a layer of pure Aluminium, this layer is a cylinder of 60 nm thickness and a radius of 400 nm:



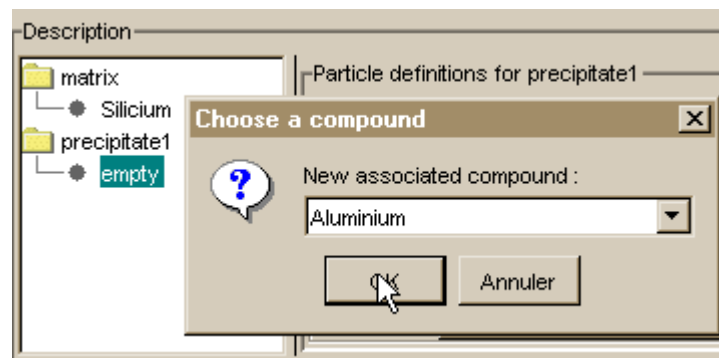
Enter the parameters as defined above, click on the cylindrical topic and enter the thickness and radius:



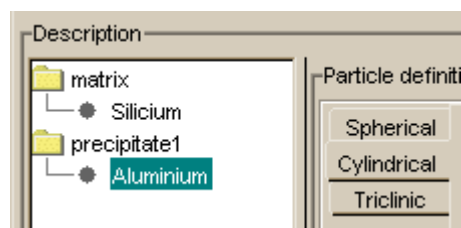
### NOTE

The origin is located in the center of the circular face of the cylinder and the Axis gives at the same time the direction and the length of the axis.

Last don't forget to select the Aluminium as the precipitate compound:



Select the Aluminium and click on OK. The new compound has replaced the empty one.



### NOTE

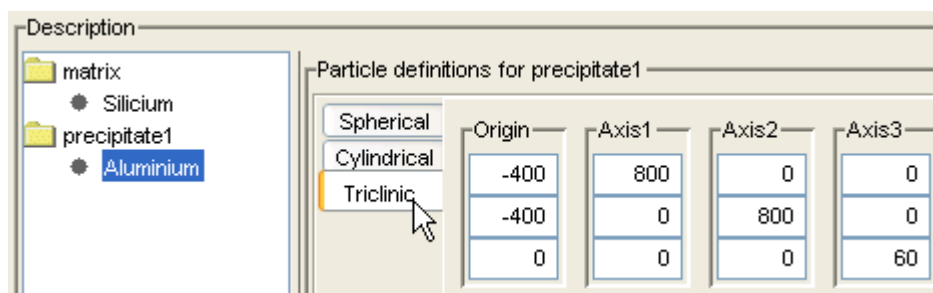
It is possible to change the precipitate name in the same way you can change compound ones.

---

## Other geometrical primitives

Two other basic geometrical objects (beside the cylinder) are available, the sphere and the rhomboedron (so-called triclinic). The sphere is easily defined by its center coordinates and its radius.

Here is the definition of a cube of aluminium of 800x800x60 nm using the triclinic object instead of the cylinder above:



### NOTE

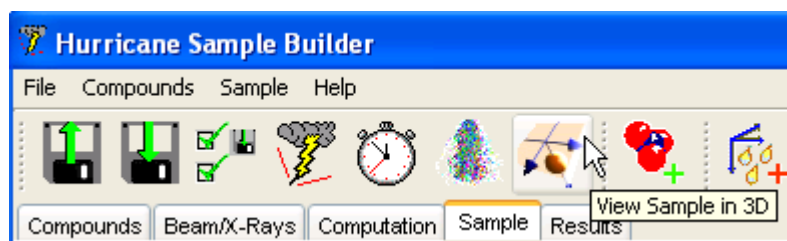
starting from the origin, the 3 axis vectors give length and direction of main edges.

# Geometry 3D view

---

## View Sample

Starting with Hurricane 1.3, the sample can be viewed in 3D. Click on the View Sample in 3D button to open the 3D window:



### NOTE

If the window is already opened, clicking on the button results in resetting the 3D view.

In the 3D window, the sample is shown from the default point of view:

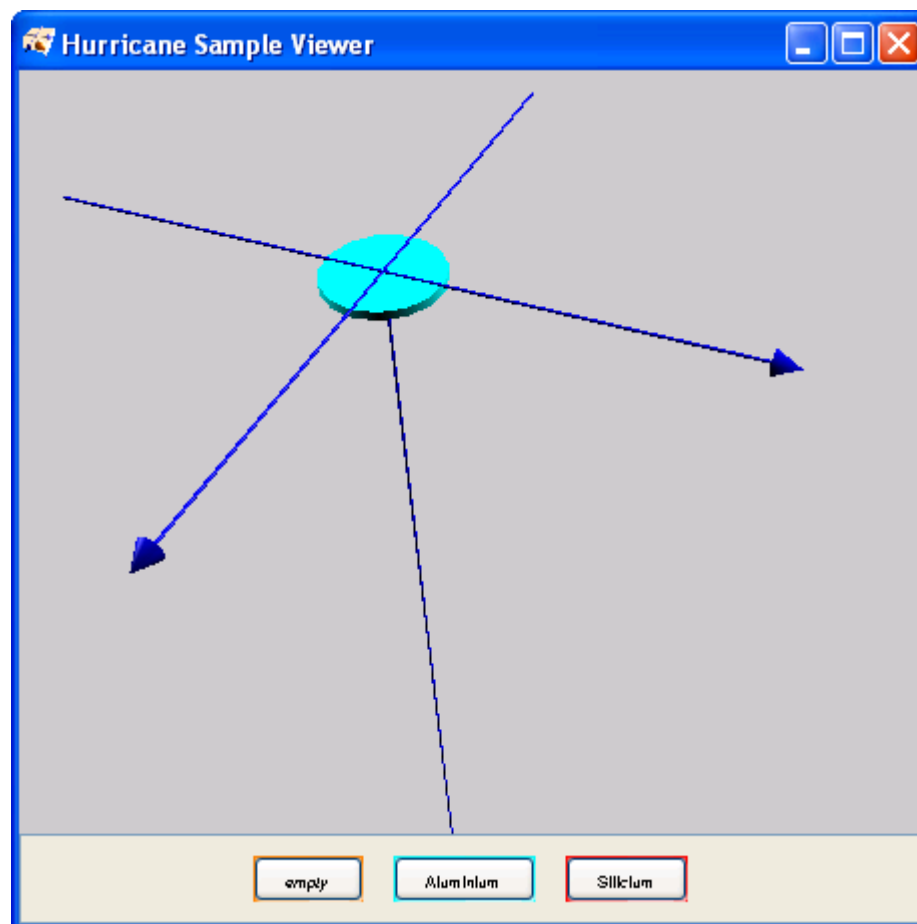
- The sample is seen from above the X-Y plane, and the Z axis is going into it (that is, deeper and deeper into the sample).
- The center of the scene corresponds to  $X=0$  and  $Z=0$ .
- The X axis is going right, and the Y axis is going down.

The view can be moved using the mouse:

- The left button allows to rotate the sample
- The right button allows sample translations.
- The mouse wheel allows zooming the sample.



Here is a possible view after using the mouse:



The 3D view can also be manipulated using the keyboard:

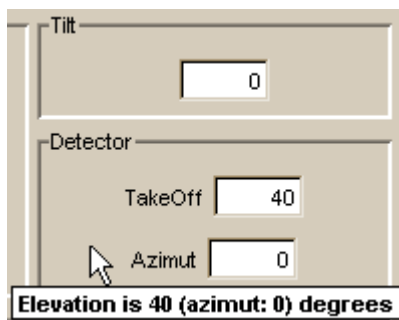
- The arrows allow rotating the sample around X and Y axis.
- The PageUp/PageDown keys allow rotating the sample around Z axis.
- Same keys combined with the Alt key allow translating along each axis.
- Same keys combined with the Shift key allow to accelerate moves.
- Plus and Minus keys allow zooming.
- Reset to default view (X-Y up front) with the Home key.

# Detector parameters

---

## The Sample Tab

The Sample tab includes a special area to enter the detector parameters as shown below:



The screenshot shows a software interface for setting detector parameters. It has a beige background with a dark border. At the top, there is a label 'Tilt' followed by a text input field containing the number '0'. Below this is a label 'Detector' followed by two more text input fields. The first is labeled 'TakeOff' and contains '40'. The second is labeled 'Azimut' and contains '0'. A mouse cursor is pointing at the 'Azimut' label. At the bottom of the interface, there is a status bar with the text 'Elevation is 40 (azimut: 0) degrees'.

### NOTE

The azimuth angle is counter clock wise or positive in the trigonometric direction. The other angles are what is usually used in an X-ray system, The takeoff angle is a positive angle above the sample and in reference to the sample plan. The sample tilt is in the trigonometric direction in the X-Z plan turning around the y axis.

# Other beam parameters

---

## Spot and Scan Modes

The Beam/X-Rays tab also includes a few other parameters:

| Mode                                  | Center                                       | Density   |
|---------------------------------------|--|---|
| <input checked="" type="radio"/> Spot | X Origin (nm) <input type="text" value="0"/> | <input checked="" type="radio"/> Uniform <input type="radio"/> Gaussian |
| <input type="radio"/> Scan            | Y Origin (nm) <input type="text" value="0"/> | Diameter <input type="text" value="1"/> nm                              |

In Spot mode, the location on the sample of the beam impact is defined in the X-Y plan. The zero is in the center of the sample, the size of the beam (density) is circular and uniform with an adjustable size.

| Mode                                  | Scanning area                                |   |
|---------------------------------------|--|---|
| <input type="radio"/> Spot            | X min (nm) <input type="text" value="-600"/> | X max (nm) <input type="text" value="600"/> |
| <input checked="" type="radio"/> Scan | Y min (nm) <input type="text" value="-600"/> | Y max (nm) <input type="text" value="600"/> |

In Scan mode, the location on the sample of the beam impact changes randomly inside a rectangular zone defined as the Scanning area while the simulation is running.

# Computation parameters

## Simulation parameters

Tab used to set a few parameters for the simulation:

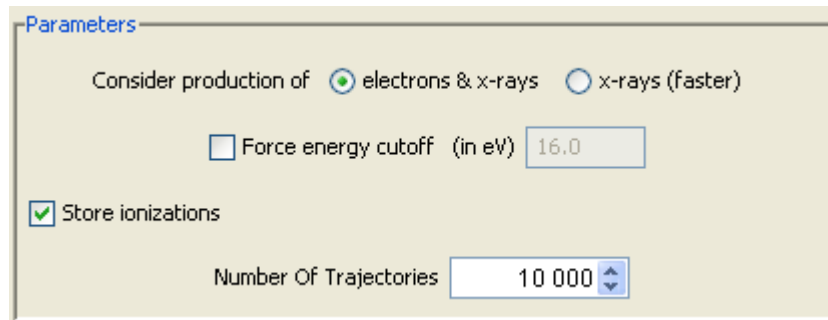
The screenshot shows the Hurricane simulation software interface with the 'Computation' tab selected. The interface is divided into several sections:

- Parameters:** Includes radio buttons for 'electrons & x-rays' (selected) and 'x-rays (faster)'. A checkbox for 'Force energy cutoff (in eV)' is present with a value of 16.0. A checked checkbox for 'Store ionizations' is shown. A 'Number Of Trajectories' spinner is set to 1 000 000.
- FileName:** A checked checkbox for 'Automatic' is shown next to the filename 'res\_A1\_Al\_S2\_Si\_15\_1000x1000x500\_10x10x10'.
- Directories:** Fields for 'Samples' and 'Tracers' both point to 'C:\Program Files\Hurricane'.
- Tracers:** A table with two columns: 'Element' and 'FileName'. It lists 'Al' and 'Si' with 'Auto' in the 'FileName' column.
- Trajectories:** Includes checkboxes for 'Store' and 'As %'. 'First' and 'Last' trajectory numbers are set to 0 and 100 respectively. A checkbox for 'Store all BSEs' is also present.

| Element | FileName |
|---------|----------|
| Al      | Auto     |
| Si      | Auto     |

The most important parameter is the number of electron trajectories used to run the simulation which for statistical reason should be kept high enough. It mostly depends on the excitation conditions; a higher beam size implies a greater number of trajectories. This number can however be reduced if you are more interested by backscattered electrons and less by ionizations.

In our example we choose 10000 trajectories.

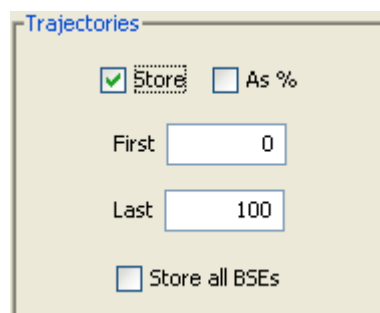
The Parameters dialog box has a title bar labeled "Parameters". It contains the following controls: a radio button group for "Consider production of" with "electrons & x-rays" selected and "x-rays (faster)" unselected; a checkbox for "Force energy cutoff (in eV)" which is unselected, next to a text box containing "16.0"; a checked checkbox for "Store ionizations"; and a label "Number Of Trajectories" next to a spin box showing "10 000".

#### NOTE

We don't recommend changing the other parameters in the same window, even for speed gain when considering only X-Rays, that is, only taking into account the electron as long as its energy is yet capable of a ionization. This will lead to an error on the backscattered electrons (of course, this may not matter if one is not interested in SE effects). In the same way, not saving the ionization will certainly reduce the memory necessary to run the simulation, but will prevent the program to calculate the emerging intensity.

Since Hurricane 1.5, it is also possible to force the energy cutoff (that is the energy threshold under which any electron trajectory is interrupted) to an higher value, mainly for speed reasons. However, the energy cutoff should not be lowered under the minimum of the energy range (this would lead to unpredictable bias in low energy elastic scattering).

Selecting the Store check box in the trajectories window will save the trajectories indicated (First, Last) in the same window. They could be displayed in the trajectory window.

The Trajectories dialog box has a title bar labeled "Trajectories". It contains the following controls: a checked checkbox for "Store" and an unselected checkbox for "As %"; a label "First" next to a text box containing "0"; a label "Last" next to a text box containing "100"; and an unselected checkbox for "Store all BSEs".

#### NOTE

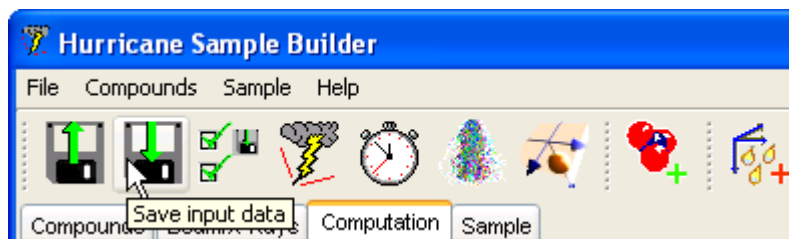
Typical values for First and Last are 0 and 100. We don't recommend to go over 300, this will considerably increase the temporary file in which we save the information.

The Directories and Tracers entries cannot be changed and are given for information. The FileName field is used to be defined when in manual input method and mainly for the batch mode.

# Saving parameters

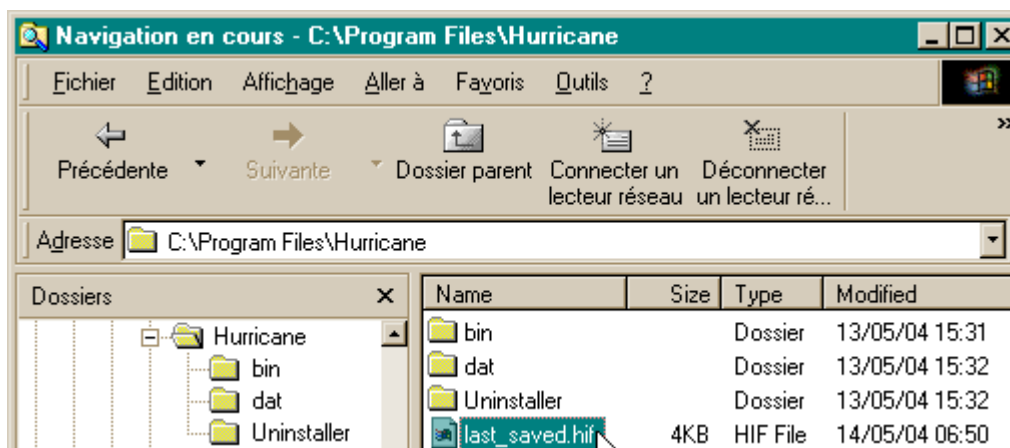
## Save configuration

To save the actual configuration and parameters, click on the save button or go through the menu ( File→Save) :



This button creates a file in the Hurricane directory:

C:\Program Files\Hurricane\last\_saved.hif

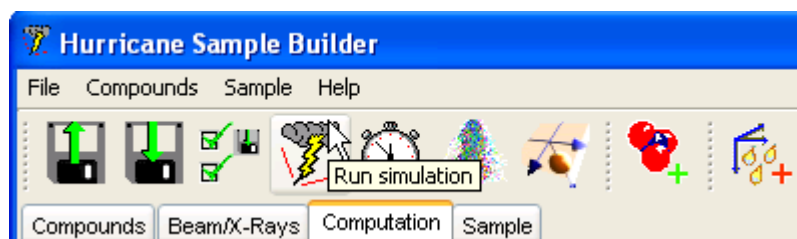


Warning: Only one set of parameters is saved in the file a new Save will erase a previous configuration.

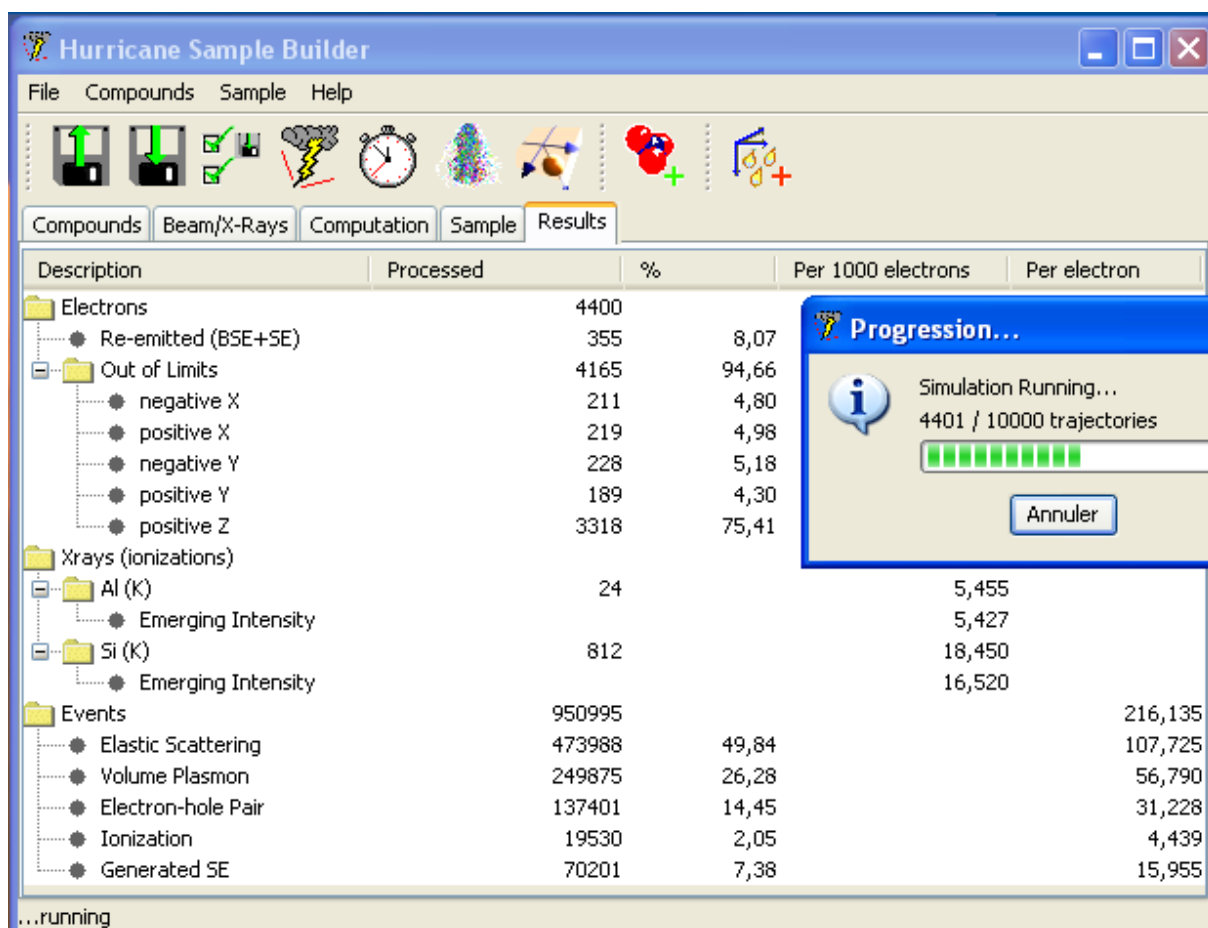
# Run the simulation

## Start simulation

Click on the corresponding button or go through the menu (File→Run) to start the simulation :



Once the computation has been started, the main window changes as follows:

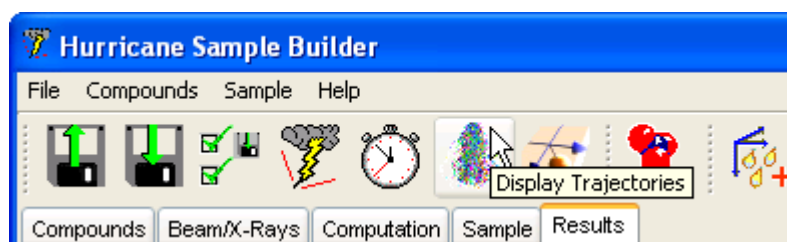




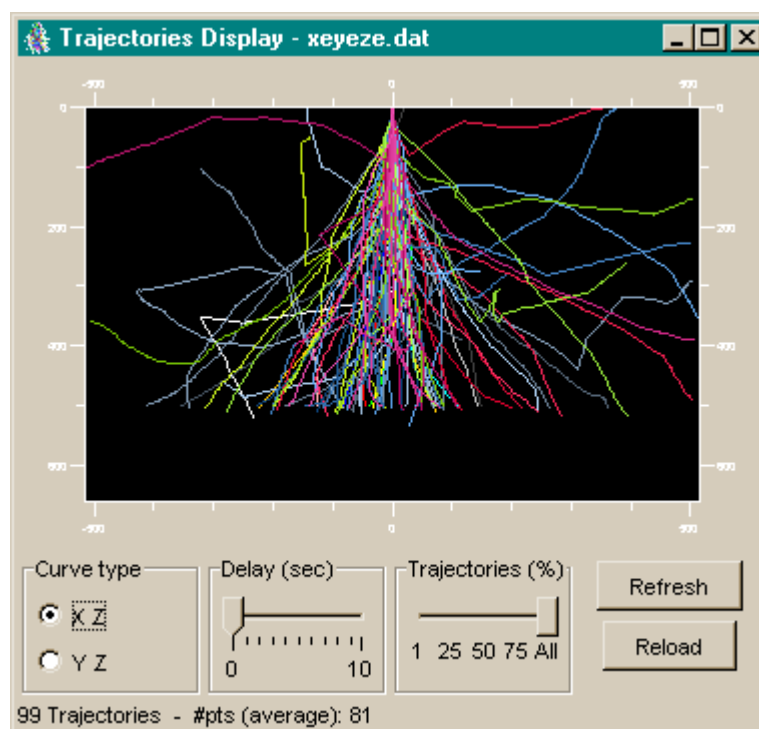
# Adjustment of the computation box

## Adjust dimension

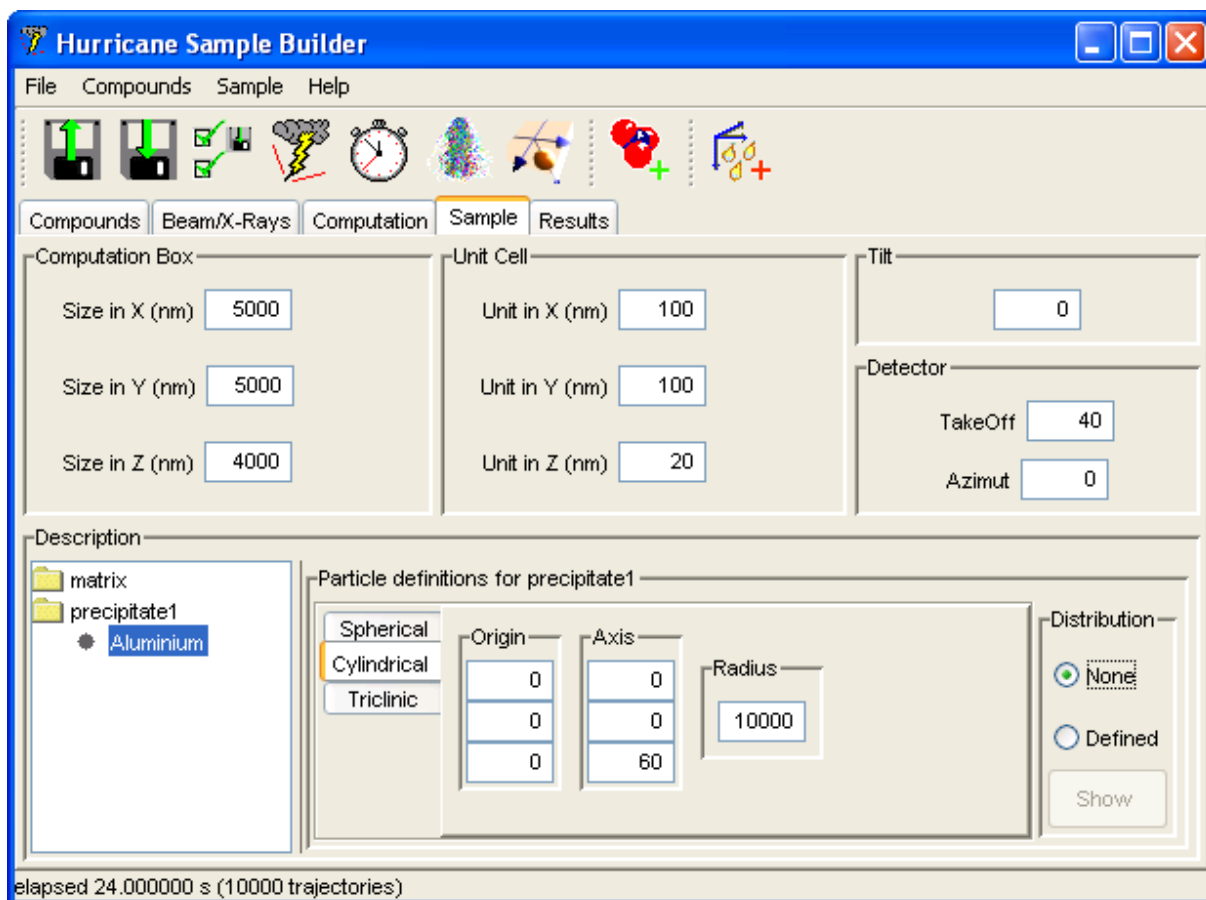
The above window shows that with the parameters we have defined most of the electrons go outside the box limits (more than 90%). This can also be seen on the trajectories display below:



Click on the Display Trajectories button



It is recommended not to go over one or two percent of the electrons outside the box. The parameters can be adjusted until the error becomes reasonable. In our example, we need to increase all sizes to define a 5000x5000x4000 volume, but we also need to increase the unit cell to, say 100x100x20, to limit the memory consumption.



### NOTE

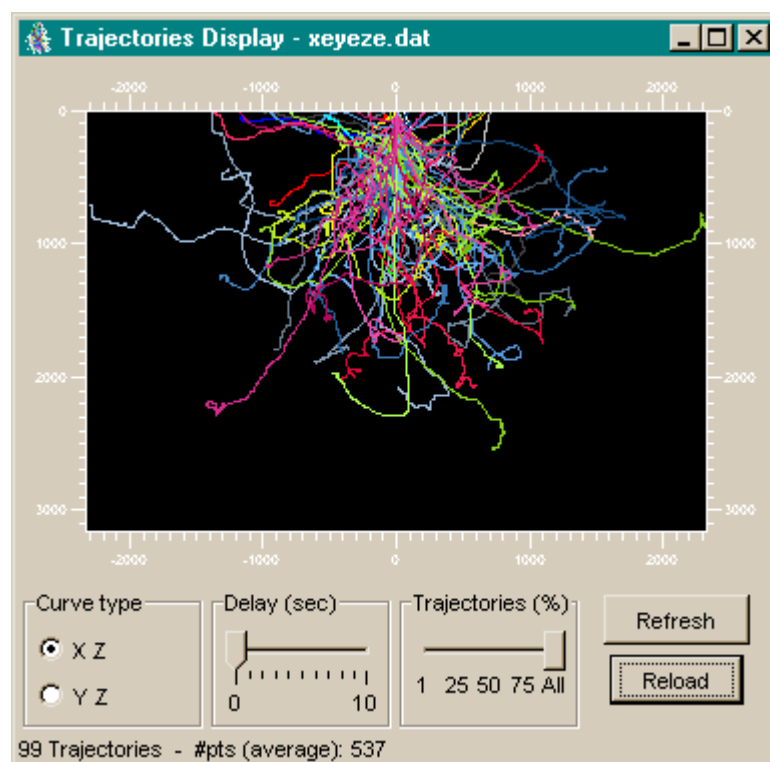
Because we had to increase X and Y size so much, we have to increase as well the radius of our precipitate as our purpose is to make it similar to a layer. After changing the radius don't forget to save the parameters again.

# Results

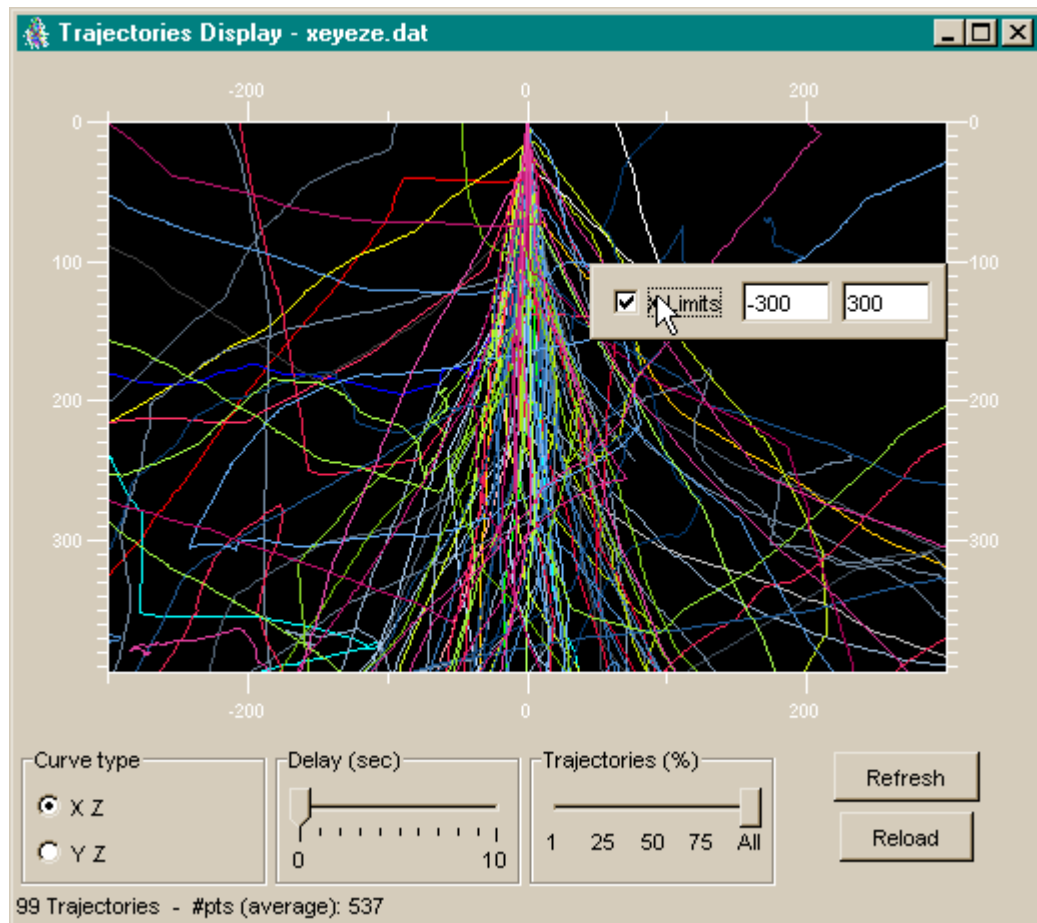
## Result windows

After this modification, here are the new result and trajectories windows:

| Compounds Beam/X-Rays Computation Sample Results |           |       |                    |              |
|--|-----------|-------|--------------------|--------------|
| Description                                      | Processed | %     | Per 1000 electrons | Per electron |
| Electrons  | 10000     |       |                    |              |
| ● Re-emitted (BSE+SE)                            | 2266      | 22,66 |                    |              |
| + Out of Limits                                  | 30        | 0,30  |                    |              |
| Xrays (ionizations)                              |           |       |                    |              |
| Al (K)   | 63        |       | 6,300              |              |
| ● Emerging Intensity                             |           |       | 6,263              |              |
| Si (K)   | 964       |       | 96,400             |              |
| ● Emerging Intensity                             |           |       | 81,030             |              |
| Events   | 14774855  |       |                    | 1477,486     |
| ● Elastic Scattering                             | 7301994   | 49,42 |                    | 730,199      |
| ● Volume Plasmon                                 | 3831114   | 25,93 |                    | 383,111      |
| ● Electron-hole Pair                             | 2243514   | 15,18 |                    | 224,351      |
| ● Ionization                                     | 272746    | 1,85  |                    | 27,275       |
| ● Generated SE                                   | 1125487   | 7,62  |                    | 112,549      |



Since Hurricane version 1.2.1, X axis display limits can be set and fixed explicitly in the trajectory window. Click on the mouse right button to have a context menu in which you can fill min and max fields and click on the X Limits check box:



Left clicking and moving the mouse while keeping the left button pressed allows dragging trajectories in the window. Rolling the (optional) mouse wheel allows zooming (however the X Limits button must be preliminarily checked).

# Ionization variance reduction

## Variance reduction techniques

The Results window below shows that less than 100 raw Aluminium K ionizations were produced, that is a very low number of events below normal statistical thresholds. It is a frequent problem as ionization events are naturally much less probable than other interaction events.

| Compounds           | Beam/X-Rays | Computation | Sample             | Results      |
|---------------------|-------------|-------------|--------------------|--------------|
| Description         | Processed   | %           | Per 1000 electrons | Per electron |
| Electrons           | 10000       |             |                    |              |
| Re-emitted (BSE+SE) | 2430        | 24,30       |                    |              |
| Out of Limits       | 34          | 0,34        |                    |              |
| Xrays (ionizations) |             |             |                    |              |
| Al (K)              | 55          |             | 5,500              |              |
| Emerging Intensity  |             |             | 5,469              |              |
| Si (K)              | 931         |             | 93,100             |              |
| Emerging Intensity  |             |             | 78,220             |              |
| Events              | 14614164    |             |                    | 1461,416     |
| Elastic Scattering  | 7227712     | 49,46       |                    | 722,771      |
| Volume Plasmon      | 3790477     | 25,94       |                    | 379,048      |
| Electron-hole Pair  | 2214338     | 15,15       |                    | 221,434      |
| Ionization          | 270433      | 1,85        |                    | 27,043       |
| Generated SE        | 1111204     | 7,60        |                    | 111,120      |

Starting with Hurricane 1.3, it is possible to use variance reduction techniques to produce more ionization events without increasing the number of trajectories thus computation time. In the Beam/X-Rays window, one can force ionization event probabilities per X-Ray line by a chosen factor (for example, apply a factor 100 for Al/K and 10 for Si/K):

|   |             |  |   |         |
|---|-------------|--|---|---------|
| Compounds                               | Beam/X-Rays | Computation  | Sample  | Results |
| <b>Accelerating Voltage</b><br>15.0 keV |             | <b>Mode</b><br><input checked="" type="radio"/> Spot<br><input type="radio"/> Scan                         | <b>Center</b><br>X Origin (nm) 0<br>Y Origin (nm) 0 |         |
| <b>Energy Range</b><br>16 eV - 30 keV   |             | <b>Density</b><br><input checked="" type="radio"/> Uniform <input type="radio"/> Gaussian<br>Diameter 1 nm |   |         |
| <b>X-Ray Lines Selection</b>            |             |  |   |         |
| Element                                 | X-Ray Lines | Variance Reduction Factor  |   |         |
| Al                                      | K           | 100  |   |         |
| Si                                      | K           | 10   |   |         |

Running again the simulation, Hurricane produces more ionization events, statistically greatly enhancing the results. Of course, excess ionization events do not play in trajectory variations,

and variance reduction factors are taken into account for raw and emerging intensity computation.

| Compounds Beam/X-Rays Computation Sample Results |           |       |                    |              |
|--|-----------|-------|--------------------|--------------|
| Description                                      | Processed | %     | Per 1000 electrons | Per electron |
| Electrons  | 10000     |       |                    |              |
| ● Re-emitted (BSE+SE)                            | 2375      | 23,75 |                    |              |
| + Out of Limits                                  | 26        | 0,26  |                    |              |
| Xrays (ionizations)                              |           |       |                    |              |
| Al (K)   | 5330      |       | 5,330              |              |
| ● Emerging Intensity                             |           |       | 5,300              |              |
| Si (K)   | 9528      |       | 95,280             |              |
| ● Emerging Intensity                             |           |       | 80,160             |              |
| Events   | 14679427  |       |                    | 1467,943     |
| ● Elastic Scattering                             | 7261895   | 49,47 |                    | 726,190      |
| ● Volume Plasmon                                 | 3808840   | 25,95 |                    | 380,884      |
| ● Electron-hole Pair                             | 2222780   | 15,14 |                    | 222,278      |
| ● Ionization                                     | 270872    | 1,85  |                    | 27,087       |
| ● Generated SE                                   | 1115040   | 7,60  |                    | 111,504      |

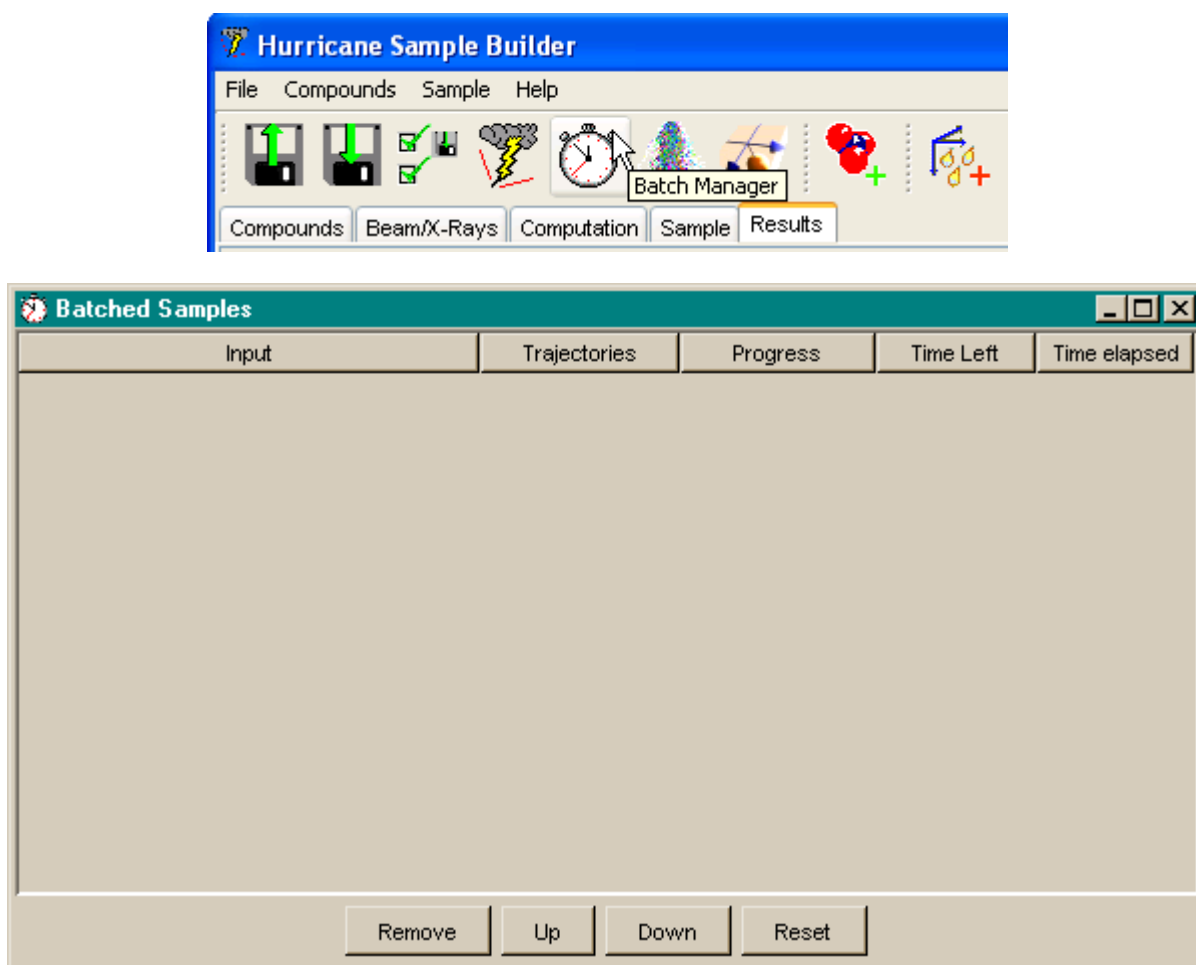
# Batch mode

---

## Introduction

The batch mode is used to automate the process so that you can run a series of samples automatically without being present.

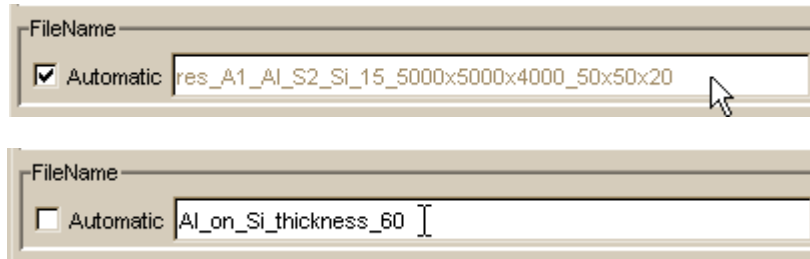
Click on the Batch button to display the batch window:



---

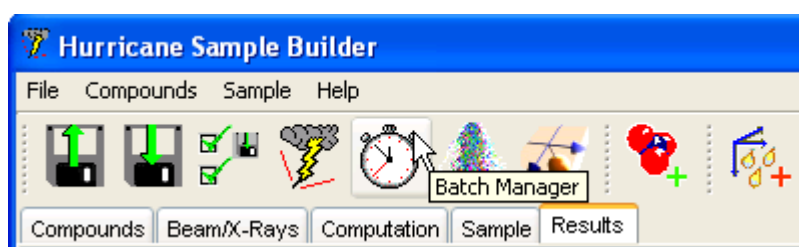
## Change the output filename

Before moving the set of parameters to the batch window, it is necessary first to change the output filename, go into the Computation tab, disable the automatic filename assignment feature and enter a specific name.



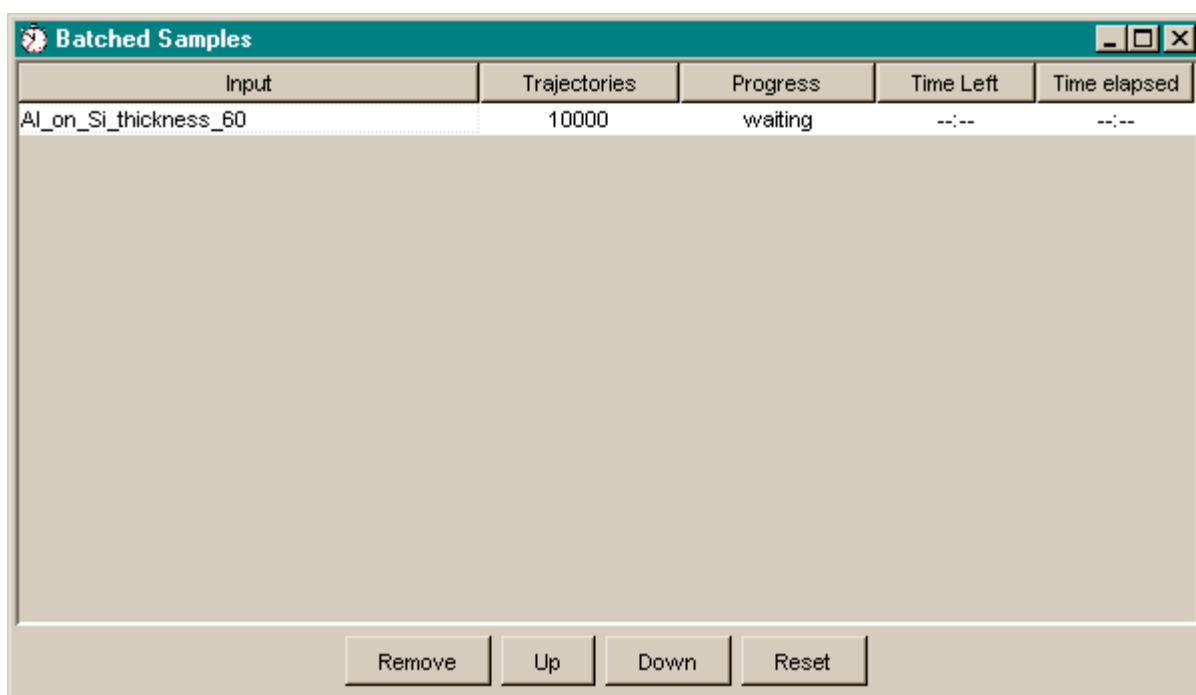


To add the parameters to the batch window click either on the batch button once more or use the menu (File→Batch):

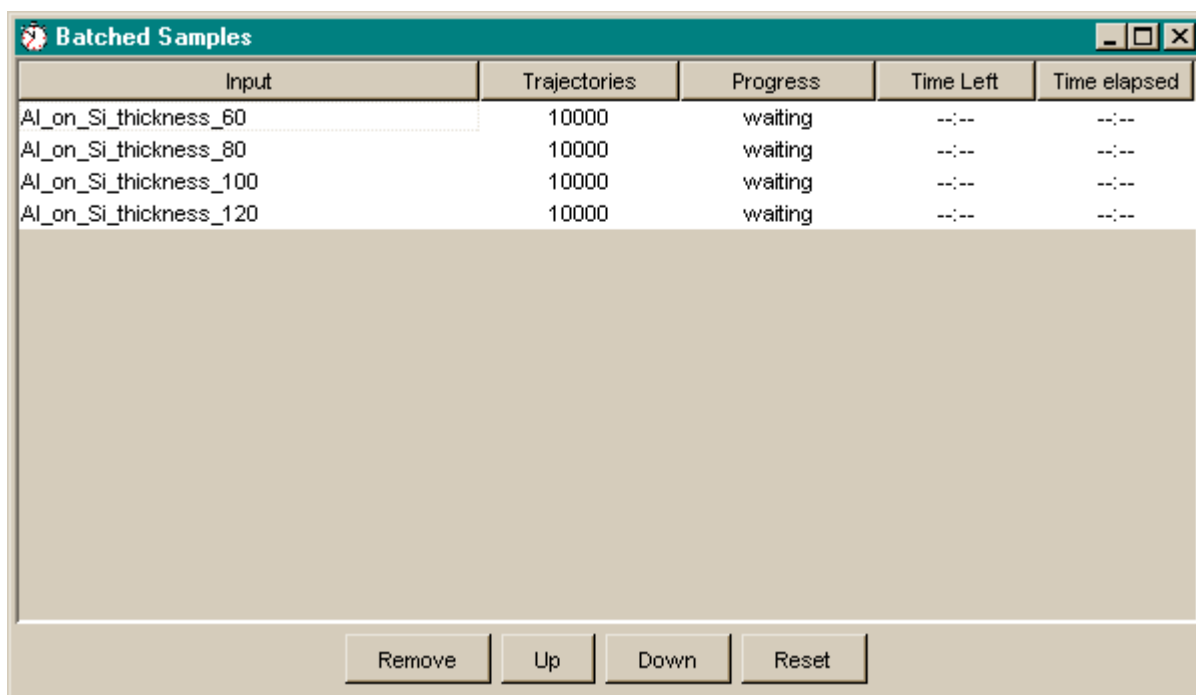


### NOTE

The effect of the batch button varies. If the batch window is closed, then pushing the button opens the batch window. If the batch window is opened, then it will add the actual parameters to the batch window.



A simple case would be to consider the same example as before with and let say, make a several batch files with different layer thickness, as shown below:

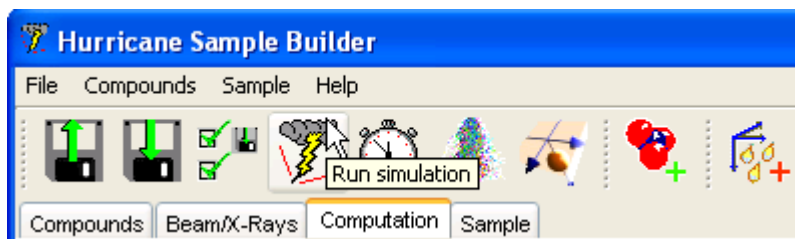


| Input                  | Trajectories | Progress | Time Left | Time elapsed |
|------------------------|--------------|----------|-----------|--------------|
| Al_on_Si_thickness_60  | 10000        | waiting  | --:--     | --:--        |
| Al_on_Si_thickness_80  | 10000        | waiting  | --:--     | --:--        |
| Al_on_Si_thickness_100 | 10000        | waiting  | --:--     | --:--        |
| Al_on_Si_thickness_120 | 10000        | waiting  | --:--     | --:--        |

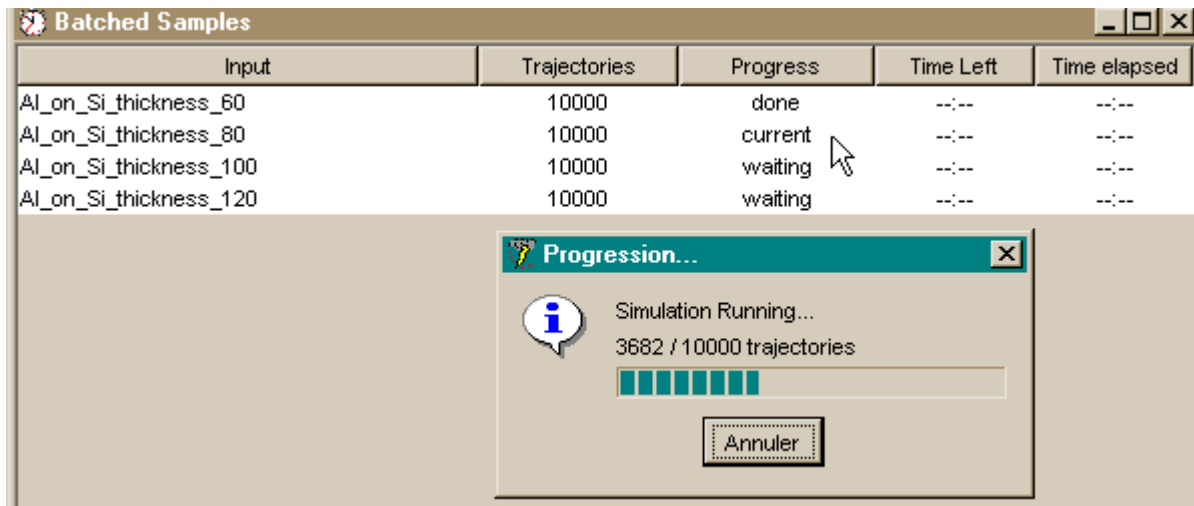
---

## Running the batch simulation

The same basic run button is used to start the batch ( File→Run) :



The program runs each file at a time:



#### NOTE

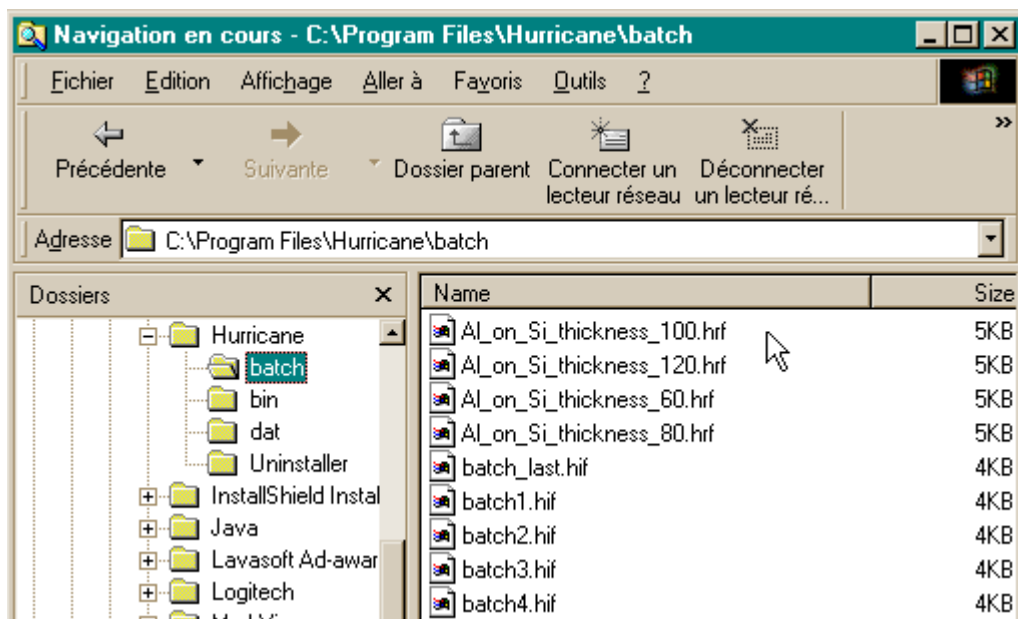
Clicking on Cancel will prompt you to either stop the all batch or to stop the actual file and move to the next one.

---

## Results in batch mode

To display the results of a particular simulation, double click on the corresponding line, the parameters of the file are then loaded into the main window. The Result tab is shown and now contains the results of this batch file.

The corresponding files have been created and saved in the directory C:\Program Files\Hurricane\batch :



#### NOTE

If the same batch simulation is ran, then the previous results file will be overwritten without being prompted.

A batch results file can be loaded by simply moving the file into the hurricane main window. A group of files can also be dropped on the Batch window to be re-computed at next batch run time.

To export the data to a spread sheet program, click on the field to be exported, one at a time, and use CTRL-C then Paste or CTRL-V in the spread sheet program.

Last to calculate the intensity ratio in the example given here, it would be necessary to run the same simulation on a standard in order to calculate the ratio of emerging intensity.

# Customize the energy range

---

## When is it needed ?

Hurricane offers as a default to take into account electron energies from 16 eV to 30 keV. While this is enough for most cases, there are at least two situations in which a custom energy range is necessary:

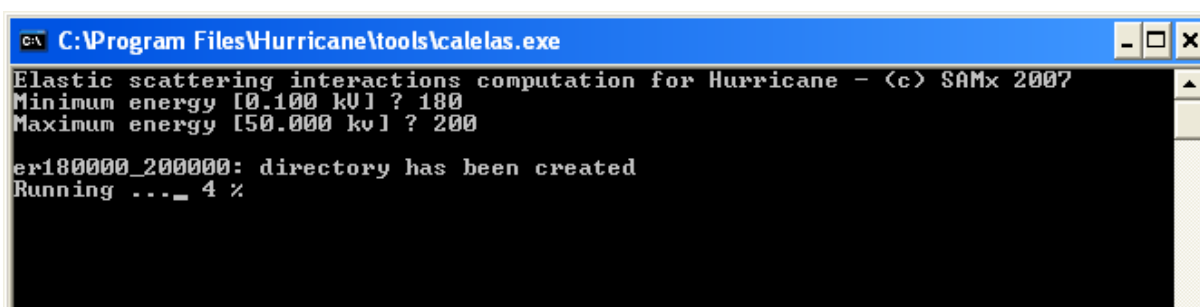
- The accelerating voltage is higher than the maximum of the available energy ranges (for example, in transmission studies).
- The energy cutoff needs to be lowered down for studying low energy electrons.

---

## Using the « calelas » tool

To define a new energy range, a unique computation step is required outside of the Hurricane interface using a special utility.

The calelas console program is available in the C:\Program Files\Hurricane\tools directory. Double-clicking runs it, then the minimum and the maximum values of the energy are asked in keV, and then the computation starts (note that it may take a while to complete, up to more than 30 minutes for high energy values). Here is an example of the computation of the range 180 keV to 200 keV, that could be used for TEM simulation on thin samples :



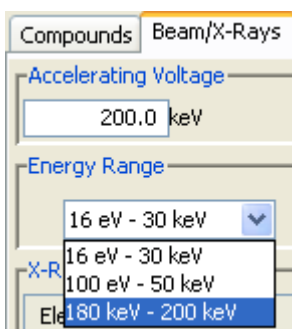
```
C:\Program Files\Hurricane\tools\calelas.exe
Elastic scattering interactions computation for Hurricane - (c) SAMx 2007
Minimum energy [0.100 kV] ? 180
Maximum energy [50.000 kV] ? 200
er180000_200000: directory has been created
Running ..._ 4 %
```

Note that the effect of running the tool is to create a subdirectory of C:\Program Files\Hurricane\dat and creating two files for each atom.

---

## Selecting a custom energy range

Once the computation has been done, the new energy range can be selected in the Beam/X-Rays tabbed window after restarting Hurricane:



# Outside Electron Classification

---

## Study the outside electrons

It has been said before that setting the right dimensions for the computation box is necessary to avoid numbers of electrons going outside. However, some users may be interested in studying these electrons going out, in which direction and with which remaining energy.

From Hurricane version 1.2, outside electrons are automatically classified depending on their direction (theta and phi angles in spherical geometry) and their final energy inside six text files. Each file includes angular and energetic distributions of electrons going outside of one computation box side.

Angles theta and phi are measured from a relative view point on each computation box plane. Each of these relative reference frames is built as a direct vector base in which the third axis is always perpendicular to the computation box side and directed to the outside. Angle phi varies between 0 and 90 degrees, it is the angular deviation from the local third axis (for example, at phi equal to 0, there is no deviation so the electron goes out perpendicularly to the computation box side). Angle theta varies between 0 and 360 degrees, it is the angular orientation of the outside electron direction projected on the computation box side. It is measured in the trigonometric (anti-clockwise) way in the local reference and the origin local first axis is always horizontal.

### NOTE

in case of a tilted sample, the local reference frames are tilted as well !

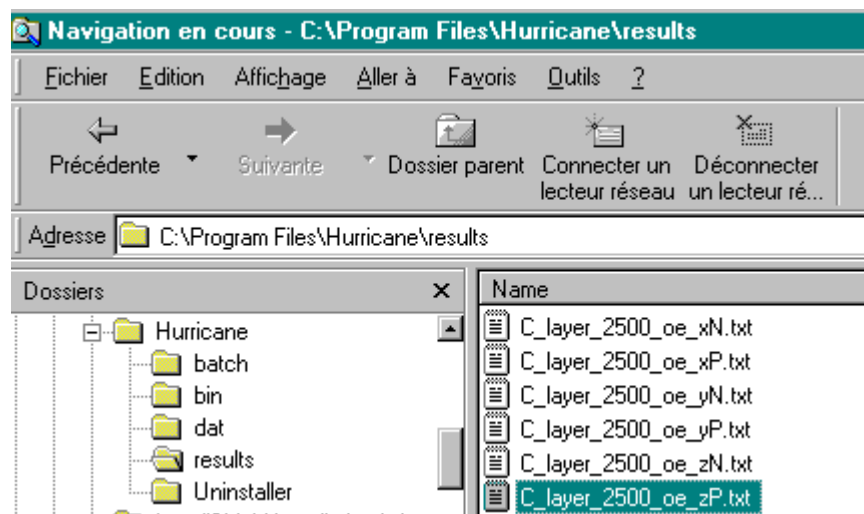
# Classification Results Files

---

## Directory result

Classification results files are found in the C:\Program Files\Hurricane\results directory. Filenames begin with the root name defined in the Computation tab and end with the \_oe\_ pattern followed by two letters giving the computation box plane through which the electron went outside (perpendicular global axis name x,y or z and direction N for negative and P for positive).

Here is an example of directory C:\Program Files\Hurricane\results contents:





# Import a Classification File in a Spreadsheet

## Results Files

As results files are tabulated text files, they can be opened inside any basic text editor :

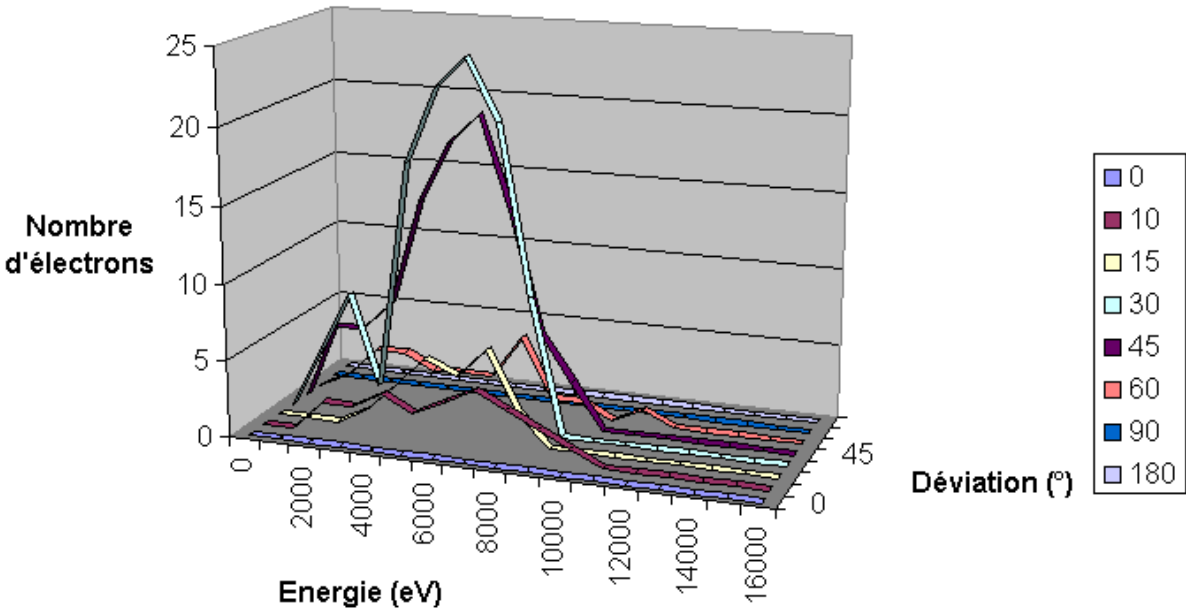
| Fichier   | Edition | Rechercher    | ?       |         |         |         |         |         |         |       |   |
|-----------|---------|---------------|---------|---------|---------|---------|---------|---------|---------|-------|---|
| theta_deg | 2       | 0.0           | 360.0   |         |         |         |         |         |         |       |   |
| phi_deg   | 9       | -180.0        | 0.0     | 10.0    | 15.0    | 30.0    | 45.0    | 60.0    | 90.0    | 180.0 |   |
| energy    | 18      | -1000000000.0 | 0.0     | 1000.0  | 2000.0  | 3000.0  | 4000.0  | 5000.0  | 6000.0  |       |   |
| 7000.0    | 8000.0  | 9000.0        | 10000.0 | 11000.0 | 12000.0 | 13000.0 | 14000.0 | 15000.0 | 16000.0 |       |   |
| theta1    | 0.0     | 360.0         |         |         |         |         |         |         |         |       |   |
| phi1      | -180.0  | 0.0           | 0       | 0       | 0       | 0       | 0       | 0       | 0       | 0     | 0 |
| 0         | 0       | 0             | 0       | 0       | 0       | 0       | 0       |         |         |       |   |
| phi2      | 0.0     | 10.0          | 0       | 0       | 2       | 2       | 3       | 2       | 3       | 4     | 3 |
| 2         | 1       | 0             | 0       | 0       | 0       | 0       | 0       |         |         |       |   |
| phi3      | 10.0    | 15.0          | 0       | 0       | 0       | 1       | 3       | 5       | 4       | 6     | 2 |
| 0         | 0       | 0             | 0       | 0       | 0       | 0       | 0       |         |         |       |   |
| phi4      | 15.0    | 30.0          | 0       | 4       | 8       | 2       | 17      | 22      | 24      | 20    | 9 |
| 0         | 0       | 0             | 0       | 0       | 0       | 0       | 0       |         |         |       |   |
| phi5      | 30.0    | 45.0          | 0       | 5       | 5       | 7       | 14      | 18      | 20      | 14    | 6 |
| 3         | 0       | 0             | 0       | 0       | 0       | 0       | 0       |         |         |       |   |
| phi6      | 45.0    | 60.0          | 0       | 1       | 3       | 3       | 2       | 2       | 2       | 5     | 1 |
| 1         | 0       | 1             | 0       | 0       | 0       | 0       | 0       |         |         |       |   |
| phi7      | 60.0    | 90.0          | 0       | 0       | 0       | 0       | 0       | 0       | 0       | 0     | 0 |
| 0         | 0       | 0             | 0       | 0       | 0       | 0       | 0       |         |         |       |   |
| phi8      | 90.0    | 180.0         | 0       | 0       | 0       | 0       | 0       | 0       | 0       | 0     | 0 |
| 0         | 0       | 0             | 0       | 0       | 0       | 0       | 0       |         |         |       |   |

The file format is very simple :

- All values are separated by tabulations.
- First three lines give class limits for the three parameters, angles theta and phi, and final electron energy.
- On each class definition line, there is an id string identifying the parameter (theta\_deg), the number of class limits, and all limit values. Extension \_deg in the id string says that angle units are degrees.
- Each counting for each energy class is lined up with others on one line beginning with the phi identifier for each phi class. Each phi limits are recalled at columns two and three.
- Each set of phi lines has got a header line beginning with the theta id string and giving theta limits in the second and third columns as well.

Such a format allows to import data easily in any spreadsheet application and to display graphics such as the following :

**Electrons transmis (C 2500 nm)**



# Classification Parameters

---

## Define classification

Hurricane uses predefined classes (1 class for theta, 16 comparable classes for phi, energy classes of 1 keV and depending on initial energy) that will not be enough in many cases. One can define its own classification following the three header line format of result files and writing it in a new tabulated text file `oe_param.txt` that must be located in the `C:\Program Files\Hurricane` directory. Moreover, it is possible to have different classes for different computation box sides creating several files `oe_param_<axis,DIRECTION>.txt` in the same directory (for example, for transmitted electrons, it is the `oe_param_zP.txt` file).

Since Hurricane 1.5, it is possible to let Hurricane compute automatically comparable classes for phi, choosing only the number of classes, and even optionally the angle range (0 to 90 degrees as default), just by not providing the detailed list of phi angles after the number of classes. Here is an example of `oe_param.txt` content to define 10 comparable phi classes between 45 and 60 degrees:

---

```
theta_deg 2 0.0 360.0
phi_deg 10_45_60
energy 17 0.0 1000.0 2000.0 3000.0 4000.0 5000.0 6000.0 7000.0 8000.0
9000.0 10000.0 11000.0 12000.0 13000.0 14000.0 15000.0 16000.0
```

---

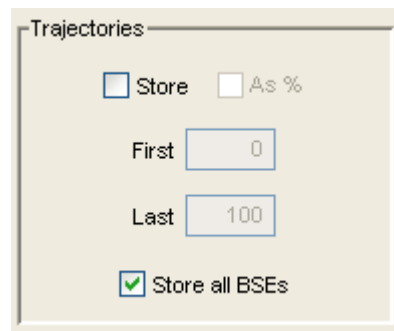
# Store all BSEs in a file

---

## In Computation tab

Since Hurricane version 1.3, it is possible to store all re-emitted electron in a simple text file.

To validate this option, go to the Computation tab and check the last checkbox in the Trajectories frame:



After running the simulation, the new output file is found in the C:\Program Files\Hurricane\results directory. The filename begins with the root name defined in the Computation tab and ends with the \_bse.txt extension. Here is an example of such a file:

| point_x_nm | point_y_nm | direction_x | direction_y | direction_z | energy_ev |
|------------|------------|-------------|-------------|-------------|-----------|
| -242,5     | 1821,2     | -0,642363   | 0,734303    | -0,219474   | 12103,8   |
| 96,5       | 64,1       | 0,035080    | 0,338049    | -0,940475   | 2592,9    |
| 1078,5     | -1008,6    | -0,150332   | -0,390328   | -0,908320   | 10615,8   |
| -200,1     | -737,7     | 0,297546    | 0,761897    | -0,575308   | 7882,6    |
| -577,6     | -125,4     | -0,725017   | -0,505554   | -0,467724   | 13895,9   |
| -47,1      | -369,1     | 0,162614    | -0,720713   | -0,673891   | 13351,3   |
| 133,7      | -533,8     | -0,686493   | 0,621534    | -0,377389   | 7819,2    |
| -574,0     | 1326,3     | -0,642889   | 0,425018    | -0,637223   | 5205,7    |
| 765,1      | 607,6      | 0,100717    | 0,556520    | 0,806577    | 6145,7    |

The text file format is very simple :

- One re-emitted electron per line.
- On one line, all values are separated by tabulations.
- The first line is an header for each column meaning: emerging X and Y coordinates in nm, normalized electron direction X, Y and Z coordinates, and electron energy in eV.