DENEB

HELP

1.28

Index

DENEB 1.28 video-demos

DENEB's YouTube videos

DENEB'S older video-tutorials

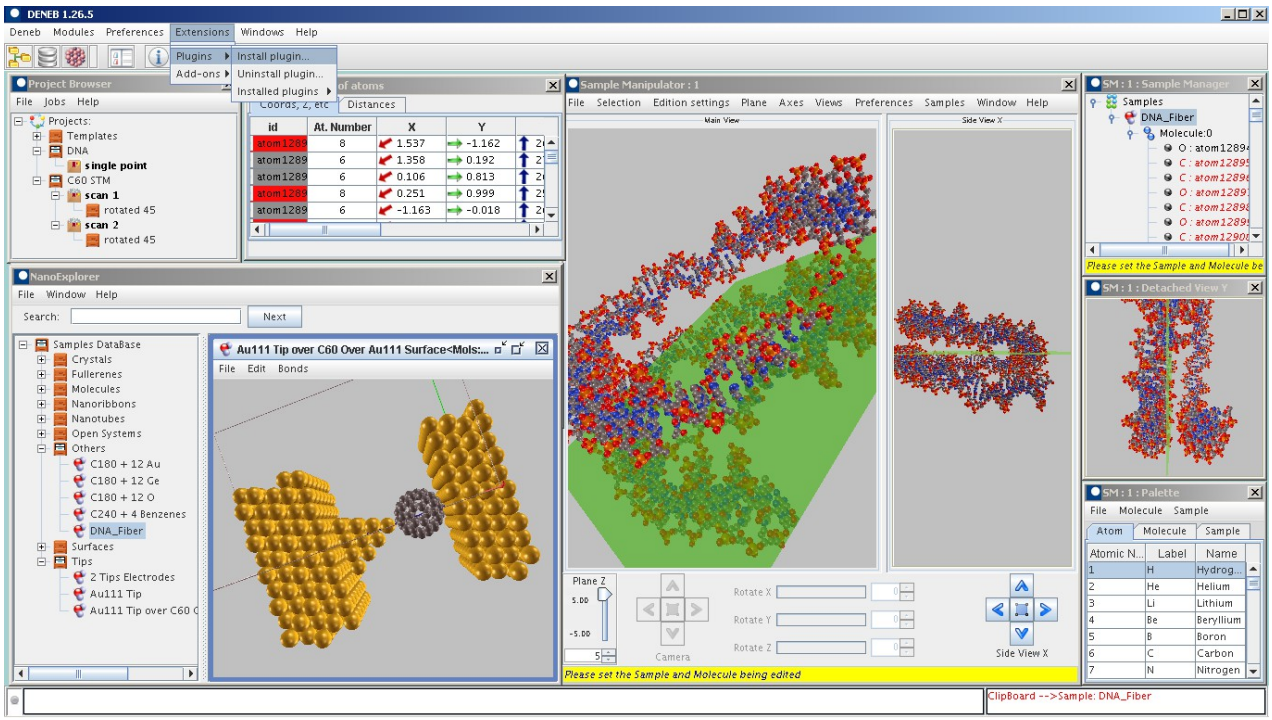
- NanoExplorer
- Project Browser
- Sample Manipulator:
  - Invoking
  - Mouse drag mode
  - Sliders and buttons mode
  - Simple building
  - Building periodic samples
- Running simulations

DENEB'S CHEAT-SHEETS

- Sample Manipulator Mouse Actions
- Sample Manipulator Key navigation

DENEB'S Known issues

DENEB's General Introduction



The philosophy behind DENEB

DENEB is a software package whose aim is to facilitate and expedite the work of researchers in the fields of *Quantum Atomistic Simulations*. With **DENEB** you can create, execute, retrieve, organize and centralize your thousands of simulations belonging to your hundreds of research projects.

Your simulations might apply to very many different physical systems, they could also belong to different *calculation engines* (e.g. **SIESTA**, **QuantumESPRESSO**, **CPMD**, **VASP**, etc), and could be launched for execution into several different remote hosts … Nevertheless, **DENEB** can keep track of each of them and present them to you neatly organized and readily accessible from your PC. Using **DENEB**´s **Project Browser** the user can choose any kind of classification for his simulations, based on kind of sample, type of calculation engine, etc. Use customary labels and organize them, in groups and projects, into tree structures of any depth. Quickly search and -with a single click- store/retrieve all of it: Simulations, projects, their organization, and their resulting data.

In a similar way, the group of all the physical systems of your interest can be easily organized using **DENEB**'s **NanoExplorer**. This tool provides with tree-organization of **thousands of samples**, fully customizable, and with *quick-search* abilities. It is seamlessly integrated with **Project Browser** and acts both as an independent database and as a source/repository of all your samples. **NanoExplorer** provides visualization and import/export abilities to/from different formats. You can *mass import your older samples*, that may be stored in different formats. Also, its whole database can be stored/retrieved with a single click.

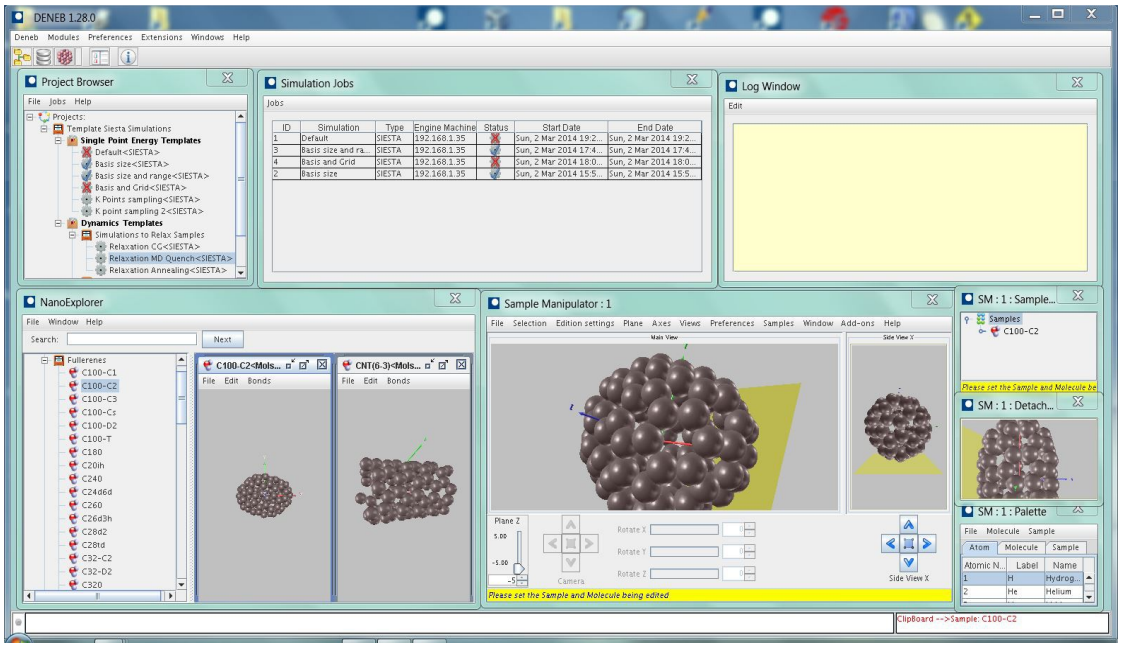
To edit your samples use **DENEB**'s **Sample Manipulator**. This tool provides with extensive abilities to build samples from scratch, combine them into new ones, and modify existing ones. With **Sample Manipulator** you have complete freedom to edit your samples in almost any imaginable way. It introduces new concepts and auxiliary graphical tools that enable accurate manipulation and navigation. You can open several instances of **Sample Manipulator** concurrently, this facilitates the simultaneous visualization/manipulation/combination of several samples. Of course, **Sample Manipulator** is also fully integrated with the rest of **DENEB**´s tools by simple copy-and-paste operations.

From **DENEB**'s **Project Browser**, you can define simulations by coupling a given sample to a given set of *computational parameters*. The **Parameter Editor** enables graphical setting of all the *computational parameters* that define the simulation. There is one **Parameter Editor** tool for each **calculation-engine plugin** (e.g. the **SIESTA** plugin, the **QE** plugin, the **VASP** plugin, etc) that you include in **DENEB**. Do not worry about what **Parameter Editor** to use on what simulation: **DENEB** keeps track of the calculation types and calls the correct editor in each case. You can use **DENEB** with *any* given number of plugins.

Project Browser's **Job Manager** is an important tool since it holds the list of simulations that have been launched, it lists their status and allows you to retrieve and access the outputs of those that have successfully finished. This tool allows you to: *Launch* simulations for execution into remote hosts where the calculation engine is installed; *monitor automatically* the remote computations' state (pending, running, success, fail); and *retrieve automatically* the computations' output-log and output files.

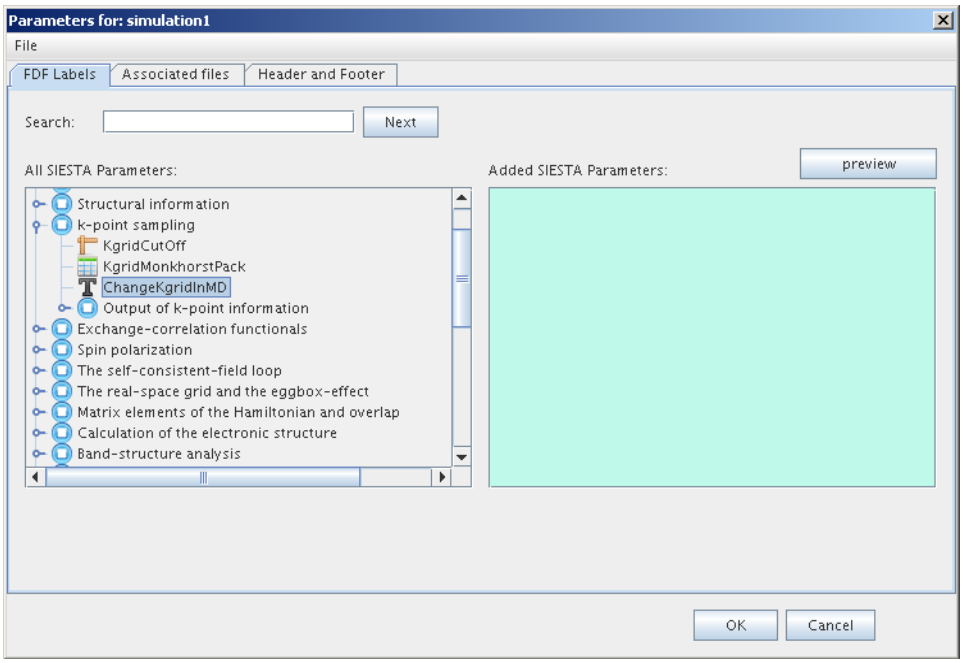
New things in DENEB 1.28 with respect to version 1.26:

1) **DENEB**'s main window menu bar has been simplified. Note that the old File menu-item in the main window referred mainly to the **Project Browser** and its projects (it had the menu items called: New project, Open project, Save project, Save project as) , so it has been moved to the Project Browser. The Exit menu item is now under a menu called Deneb. You can still access **Project Browser**, **NanoExplorer** and **Sample Manipulator** from the Modules menu. The menu item called Preferences contains the old Edit – Preferences menu item plus a new menu item called Edit File formats, which is used to define how **DENEB** will automatically plot 2D graphs as a function of the file extension (this applies to the new XY-plotter addon).

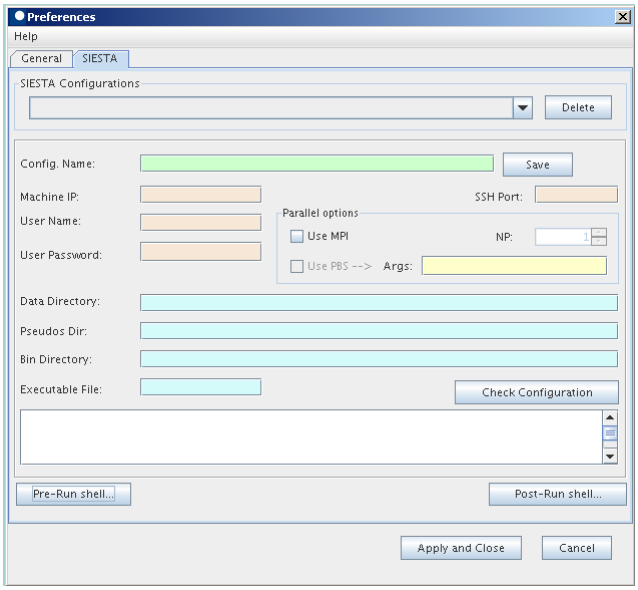


2) The **siesta Parameters Editor** has been quite improved. You can now easily save and recover your favorite set of default values for all fdf labels, use for that purpose the new menu items called File → Load template , and File → Save as template. The latter will store in a file your whole set of current fdf labels (added or not) and the former will recover them. This way you can quickly load you set of default values for your fdf labels as you have them stored in a file. Another obvious new feature is the addition of two new tabs:

- Associated files. In this tab you can choose one or multiple files that will be sent to the calculation engine machine just before launching the remote jobs. You can this way send files that might be sought for by siesta when executing.
- Header and footer. In this tab you can add any text that you consider at the top (header part) or the bottom (footer part) of the generated engine input file. For example if you have added to siesta your own fdf labels (they are not therefore found in the tree of the Parameters Editor) you may add here their definition and values. The effect is as if you type the corresponding text on the top (and bottom) of the automatically generated fdf file that will be sent to the calculation-engine. You can also use this to add your extended comments or explanations about a particular engine file. Last, but not least, **DENEB** 1.28 comes with tooltips explanation of each fdf label, in case your memory needs refreshing about a particular label, just place the cursor over any of them and see the text appearing.



3) In the Siesta engine configuration now you can freely define what bash shell commands will be run before and after the launching of the Siesta simulation. This way one can easily, for example, load MPI modules if needed. Use with care as any command would be run and there are potentially destructive uses of this features. Note the new buttons called Pre-Run shell... and Post-Run shell... The interface for the engine configurations definition has been improved as well.



4) A number of fixes and other improvements have been put in place, it is suggested therefore to update to 1.28 for users of older versions of **DENEB**.

Installation of DENEB and plugins

DENEB TRIAL installation instructions

To install **DENEB** Trial in your PC is very easy, you only have to follow these steps:

- **For Windows** (7, Vista):
  1. Download and execute the latest **DENEB** installer for Windows, trial version, for example: "`deneb_TRIAL_1.28.0-setup.exe`".
  2. Follow the instructions from the installation wizard.
- **For Linux** (most recent distributions):
  1. Download and execute the latest **DENEB** installer for Linux, trial version, for example: "`deneb_TRIAL_linux_1.28.0-setup.bin`". You might need to set execution permission to the file.
  2. The installation will proceed automatically. Execute `./run.sh` from the installation directory, to launch **DENEB**. You can optionally execute the shell called `createShortCut.sh` so that **DENEB**'s icon will appear in the launcher when executing it.

DENEB FULL installation instructions

To install **DENEB**-Full in your PC is as easy as with the Trial version, and proceeds in the same way, but requires an extra step: At the end of the installation a file called `deneb.post` (just a few bytes with the hardware fingerprint) will be produced. Send this to `support@atelgraphics.com` so we can produce and send you back your node-locked license files. Those files (typically `deneb.lic` for **DENEB**-core, plus the plugin-related license files: `psiesta.lic` for example) just have to be placed in the same directory where you found deneb.post, so that Deneb can find them at execution time.

Hardware minimum requirements to successfully run **DENEB**:

- Intel i3 CPU 2.4 GHz or better. Or AMD equivalent CPUs.
- 3 Gb RAM.
- 150 Mb available hard disk space.
- Graphics card ATI Mobility Radeon HD 5145, or better, with 1 GB Graphics Memory, with the latest drivers.

Note: **DENEB** can run in less powerful hardware configurations, but good real-time response might not be obtained under those circumstances.

Hardware suggested requirements for a very good performance:

- Intel i7 920 2.6 GHz or better. Or AMD equivalent CPUs.
- 4 Gb RAM or greater.
- 150 Mb available hard disk space.
- Graphics card Nvidia GT220, ATI 5570 or better with 2 GB Graphics Memory, with the latest drivers.

Supported Operating Systems:

- Windows vista/ windows7 with .NET framework 3.5 or better with latest service packs and the latest drivers (DirectX 10 or newer).
- Linux Kernel 2.4 or newer.

Installing a plugin in **DENEB**

In order to create simulations and run them in your Engine, you need to **install the plugin** corresponding to the calculation engine (e.g., **SIESTA** or **CPMD** or **VASP**). This is how to install a plugin in **DENEB**:

- 1.- Download *a plugin file* (with extension **`.bin`**) for your Engine from the Atelgraphics website.
- 2.- Obtain from Atelgraphics your plugin license file.
- 3.- Run **DENEB** application.
- 4.- Select **`Plugins->Install plugin`** from the **Main menu**.

- 5.- Browse and select your downloaded **.bin** file and press the **`Apply`** button.
- 6.- Put in **DENEB**'s root directory your plugin license file.

Notes:

- **DENEB** TRIAL version comes with the SIESTA plugin **already** installed. So, out of the box, you can produce and launch siesta calculations from **DENEB**'s Project Browser with a single click.
- Do not hesitate contacting us at: `info@atelgraphics.com` reporting non expected behaviors of **DENEB**.
- Make sure that you have installed the latest drivers for your graphics card. This is relevant specially in Linux since **DENEB** might not work properly unless you make sure that you have installed some recent drivers. To achieve this, it sometimes requires for you to access the manufacturer web-page, download the drivers, and manually install them.

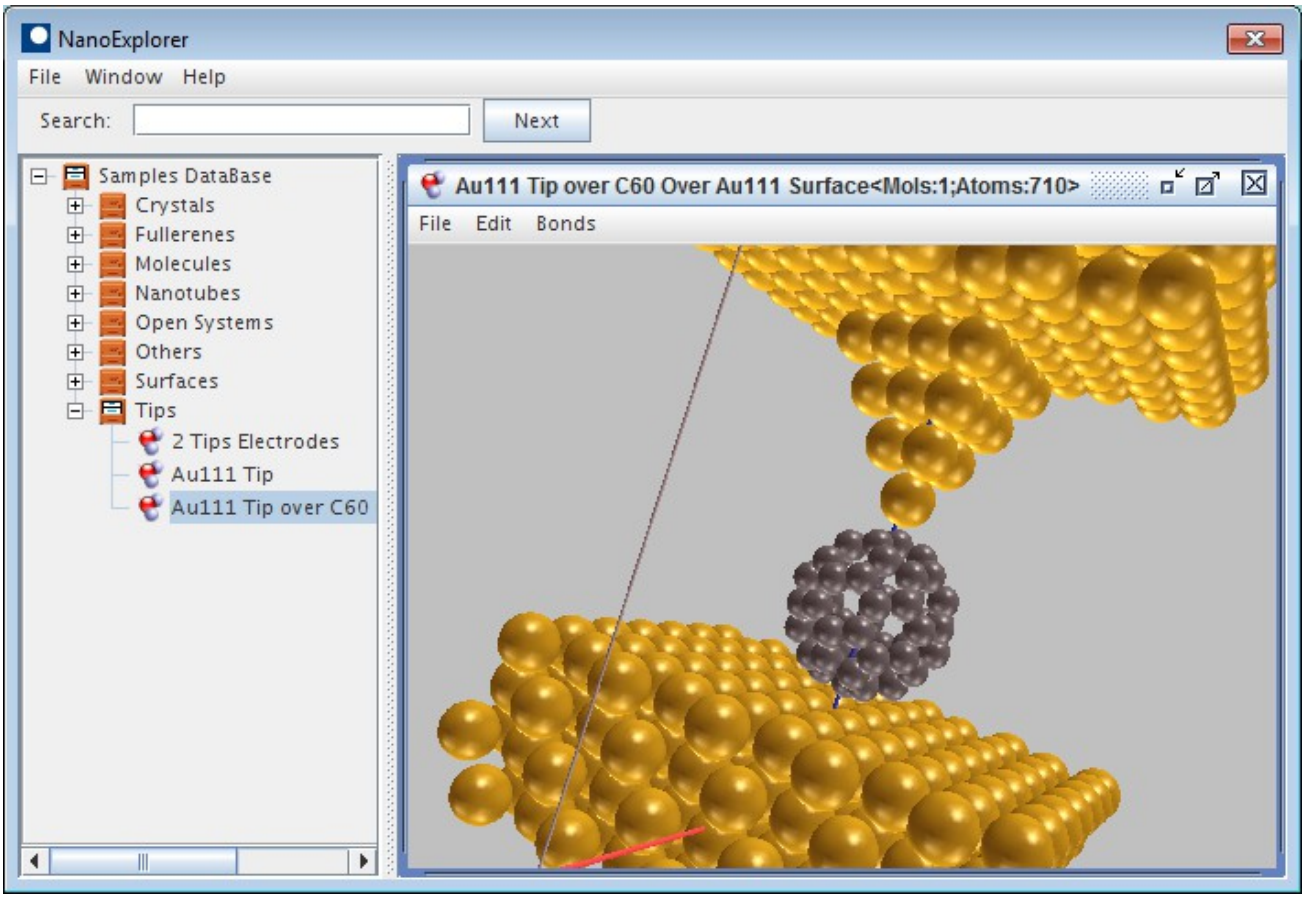
Atoms, molecules and samples in DENEB

For DENEB, the **sample** is the basic unit that specifies a physical system. A sample is part of a **simulation.** In other words, we only need to couple a sample with a *set of computational parameters* in order to completely define a given simulation. Briefly defined: **A sample is a set of molecules**. In turn, **a molecule is simply defined as a set of atoms**. And an **atom** is defined as a given nucleus placed at a given point of space. As for the electrons: To define a given sample, electrons need not to be specified since the electronic density is, instead, usually a result of the simulation once computed.

Atoms are represented as spheres in DENEB. By default their size is given by the covalent radius of the corresponding chemical specie. Their default color is given by some common standard (JMol). The radii and colors of any group of atoms can be customarily changed at will, when using **Sample Manipulator.**

Molecules and samples do not have any particular representation on their own, other than their group of atoms (spheres). You can, nevertheless, select/unselect, translate, rotate, replace, eliminate, etc, in short, treat them as units by using the **Sample Manager** of **Sample Manipulator.** Samples and molecules can also be addressed by mouse actions if choosing the pick mode accordingly (pick mode options are: 'atom', 'molecule' and 'sample'). You can also clone them (or parts of them) and transfer molecules from sample to sample, or atoms from molecule to molecule, etc... the very many possibilities will be discovered in this document and video-tutorials.

DENEB's NanoExplorer



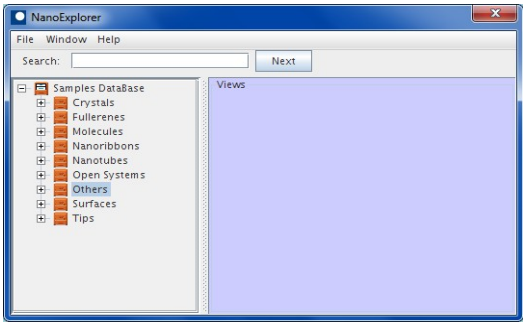
DENEB's NanoExplorer: Loading new samples

As we have said in previous sections, for DENEB, the **sample** is the basic unit that specifies a physical system. DENEB's **NanoExplorer** is a database of samples, that may contain any number of samples organized in groups in an arbitrary tree structure. The samples in **NanoExplorer** can be used as the starting point, or building blocks to compose new samples using **Sample Manipulator**. In addition, any new sample built in **Sample Manipulator** can be stored for later use in **NanoExplorer**. The connection point among these tools and the **Project Browser** is, as you already know, DENEB's **Clipboard**. Out of the box **NanoExplorer** comes filled out with some samples in some default tree structure, importantly, note that these are just some examples on how you can organize your **NanoExplorer** database, they are not meant to be accurate or useful for any particular purpose. **NanoExplorer** is instead intended to be your private set of own tested samples.

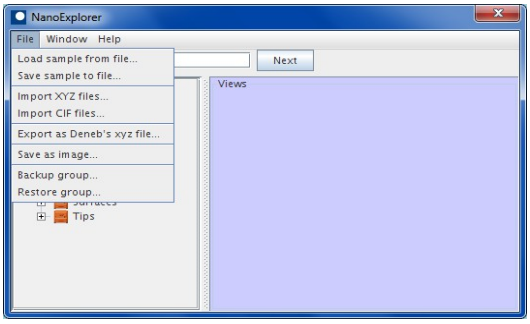
We show next how to load samples into **NanoExplorer**. There are several ways:

1) Using **NanoExplorer**'s Load Sample from file ... menu item. This is used to load into **NanoExplorer** samples that have been stored in files using DENEB's native format (extension `.dns`). This is the procedure:

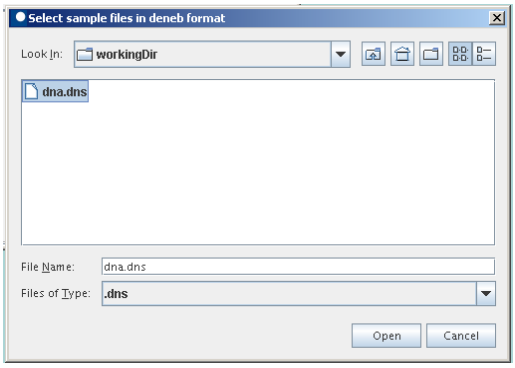
   (a) From DENEB's main menu bar choose: Modules → NanoExplorer. This will raise or show **NanoExplorer** if hidden.
   (b) Select one of the groups in **NanoExplorer**, the loaded sample will be added to the selected group.



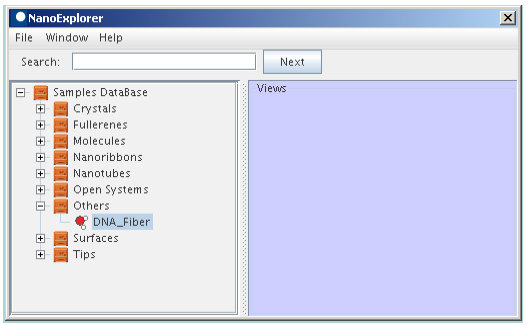
   (c) Select File from **NanoExplorer**'s main menu.



   (d) Select Load Sample from file ... A new dialog for the selection of the file appears.
   (e) Choose or type the name of the file that you want to load into **NanoExplorer**. It should be a file with extension .dns (a sample in native DENEB's format).

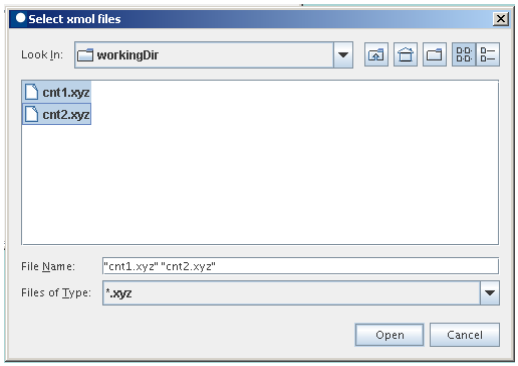


(f) Check that it has been loaded into the selected group. Note that the name of the new sample in **NanoExplorer** need not to coincide with the name of the file. Likewise you can save any sample labeled "x" in a file named "y", these names could, but need not, be the same.

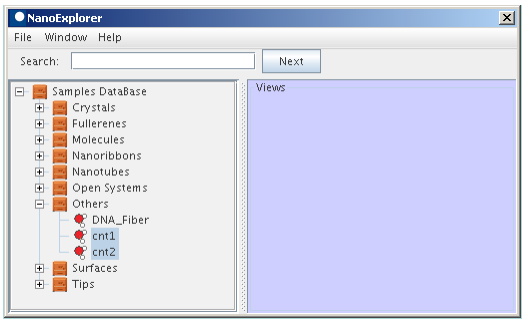


2) Using **NanoExplorer**'s Import XYZ files ... menu item. This is used to load into **NanoExplorer** files that have been stored in the `XYZ` simple format (extension **`.XYZ`**) **`[1]`**. This is the procedure:

(a) Follow steps a, b and c of the previous case (called: using **NanoExplorer**'s Load Sample from file ... menu item).
(b) Select Import XYZ files. A new dialog for the selection of files appears.
(c) Select one **or several** files to be loaded. You can either select them with mouse actions or type their file names subsequently between double quotes and separated by white spaces. Click `Open`.



(d) Check that the files have been loaded. In this case the name of the samples in **NanoExplorer** is directly taken from the name of the file. This is because the simple **`XYZ`** format does not include any label for the sample it contains. You can later on rename the sample as you wish using its context menu (triggered by `Right-Click` on the highlighted item).
(e) Optionally, visualize the samples contained in the just loaded files by using their `context menus`. Select, for this purpose, Visualize Sample. To pop out the context menu of a given



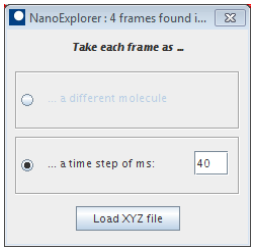
sample you have to highlight it first and then `Right-Click` on it.

(f) If the file to be loaded holds more than one set of atoms, i.e. it consists of the concatenation of "single configurations" in the `XYZ` format, a choice menu will appear in which the user can choose between two options, load each frame as:

- ... as different molecule

or

- ... as a time step of ms



When the button Load XYZ File is pressed, the file will be loaded using the currently selected choice. This way, one can use the `XYZ` format files either to describe a single sample composed of several molecules or a single sample that evolves in time. In the latter choice **DENEB** will firstly check that all frames are consistent (they have the same chemical species in the same order), and then, **DENEB** will produce an animation where from frame to frame a pause of the chosen number of mili-seconds (the default is 40) will be taken when it is played in the automatic mode (automatic animation can be played using **Sample Manipulator**). Note: If a sample contains an animation, we usually say that it contains a trajectory.

Notes:

- The icon representing the sample in the **NanoExplorer** tree denotes if it contains a trajectory, in such case this is how it looks:

- If **DENEB** detects that the frames do not belong to the same sample, it will not be loaded, in this case an error message will be written in **DENEB'S Log Window**, such as: "`ERROR:(...):(...):the frames do not belong to the evolution of the same sample`"

1) Using the following **NanoExplorer**'s menu items:
   - Import CIF files,
   - Import FDF Files,

is analogous to the previously explained section about the menu item called Import XYZ files, therefore we will not repeat the details here.

[1] Note about the `XYZ` format. In this simple format the list of atoms is given as the chemical species symbol followed by the coordinates of the atom in Angstroms. There is a header consisting of

two lines: the first line contains only the number of atoms, while the second line is an arbitrary comment that can be left blank eventually (but can not be removed). In this format one can subsequently attach one set of atoms after another in the same file. **DENEB** can load these "multi-frame files" doing the interpretation of each set **either** as a new molecule of the same sample, **or** as a new frame (*instantaneous photo* or *time step*) of the **dynamics** of a given sample. Use **Sample Manipulator** to open multi-frame `XYZ` files selecting one of these options, note that when you select to load a multi-frame `XYZ` file as the dynamics of the same set of atoms, one requisite, that **DENEB** checks for, is that all frames refer to the same set of atoms at different times, i.e. The number of atoms should coincide for all frames, and the chemical species should also coincide from one frame to the next. These conditions need not to be met when the file is loaded using the other modality: that of considering each frame as a different molecule of the same sample. A last note about the `XYZ` format as understood by **DENEB** is that *one can use the comment line to instruct **DENEB** with useful information*. In particular one can define the `Unit Cell` of the sample in such comment line (or the comment line corresponding to the first frame in the case of multi-frame files). To achieve this, simply write the unit cell lattice vectors in the comment line as follows: `latticeVectors:[ ax ay az#bx by bz#cx cy cz ]` being (ax,ay,az) the coordinates of the first lattice vector ins Angs (replace ax by the corresponding number, etc), (bx,by,bz) the coordinates of the second, and so on and so forth. This way, the so called "**DENEB**'s **XYZ** format" is compatible but extends the capabilities of the standard **XYZ** format. Here is a verbatim example of a multi-frame file in **DENEB**'s **XYZ** format:

```
3
latticeVectors:[ 5.0 0.0 0.0 # 0.0 7.0 0.0 # 0.0 0.0 6.0 ]
O    0.0   0.0   0.0
H    0.8   0.0   0.0
H   -0.2   0.7   0.0
3

O    0.0   0.0   1.0
H    0.8   0.0   1.0
H   -0.2   0.7   1.0
3

O    0.0   0.0   2.0
H    0.8   0.0   2.0
H   -0.2   0.7   2.0
3

O    0.0   0.0   3.0
H    0.8   0.0   3.0
H   -0.2   0.7   3.0
```

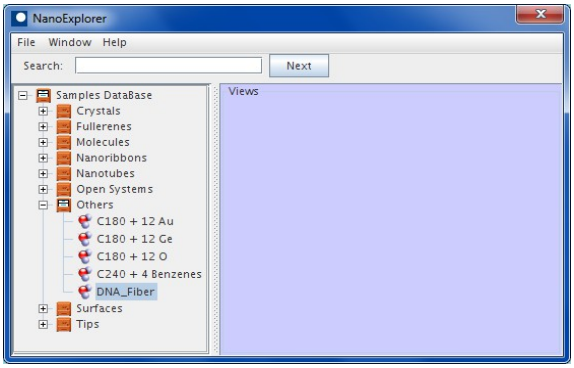
It contains four frames that represent the same set of atoms with the only difference that are displaced by one Ang along the Z axis from one frame to the next. Therefore in this case you could optionally load (using **Sample Manipulator**) this file as a time series or as a series of molecules that belong to the same sample.

DENEB's NanoExplorer: Saving samples

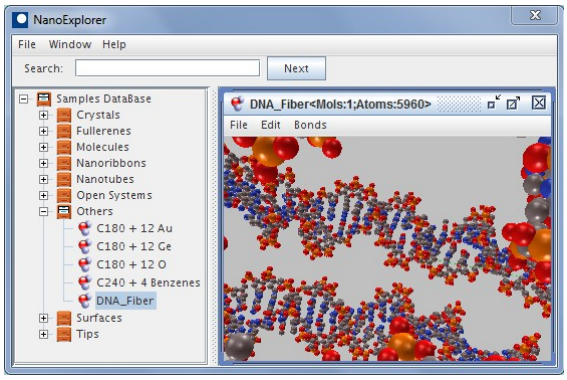
As we have said in previous sections, for DENEB, the **sample** is the basic unit that specifies a physical system. DENEB's **NanoExplorer** is a database of samples, that may contain any number of samples organized in groups, in an arbitrary tree structure. The samples in **NanoExplorer** can be used as the starting point, or building blocks to compose new samples, when using **Sample Manipulator**. Also, any new sample built using **Sample Manipulator** can be stored for later use in **NanoExplorer**. The connection point among these utilities and the **Project Browser** is, as you already know, DENEB's **Clipboard**. Out of the box **NanoExplorer** comes filled out with some samples in some default tree structure, importantly, note that these are just some examples on how you can organize your **NanoExplorer** database, they are not meant to be accurate or useful for any particular purpose. **NanoExplorer** is instead intended to be your private set of own tested samples.

We show next how to **save in disk** the samples stored in **NanoExplorer**. There are several ways:

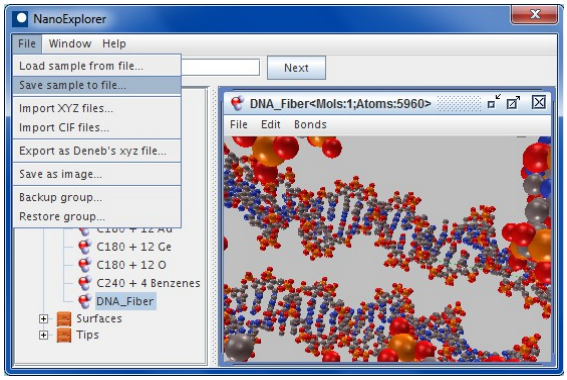
1) Doing nothing at all: ***NanoExplorer** has file persistence built in*, this means that, every time you add a new sample to **NanoExplorer**, it will create a related file and will store the information in there. It acts as a persistence database in this sense. You can close DENEB at anytime being sure that all samples in **NanoExplorer** will remain there next time when you open DENEB. **NanoExplorer** is, in fact, the standard place where you will give persistence and organization to all your samples when using DENEB. It can hold hundreds of thousands of samples, and it implements lazy loading algorithms; this means that you do not need to worry about the size of the whole database in **NanoExplorer**. Even though the data base might be too large in terms of memory, DENEB only loads in RAM the samples that are being used at each time, while the rest remain stored in disk.
2) Using the Save Sample to file... menu item from **NanoExplorer**'s File menu.
   (a) Highlight the sample that you intend to save.



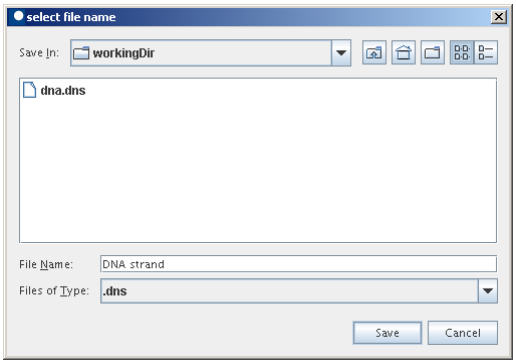
   (b) Optionally. Use its context menu (trigger the context menu by `Right-Click` on the highlighted sample) to visualize it. So you can be sure that it is, in fact, the one that you want to export. The corresponding **view window** lets you know the **number of molecules** and the **number of atoms** that the sample contains, it can be seen in the title bar of the same.



(c) Select File from the **NanoExplorer** menu bar, choose Save Sample to file ...



(d) A new dialog appears to let you choose the file name where the sample is going to be saved in **DENEB**'s native format. Choose the file name by mouse actions or type a new name. Click "Save".

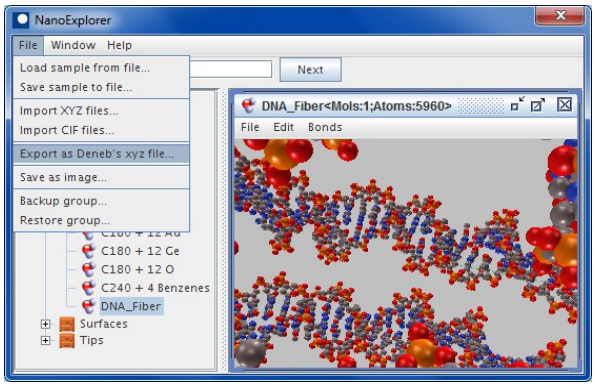


(e) This completes the process, you can **verify** that the sample has been correctly saved in that particular file by reloading it into **NanoExplorer,** into a different group to avoid confusion. But note that there would not be name collisions as ***NanoExplorer*** *admits name redundancy*.

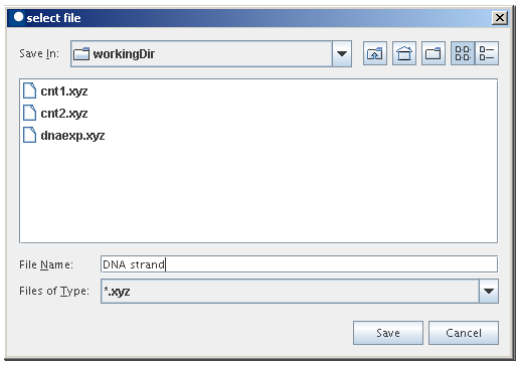
3) Using the Export as DENEB XYZ file. menu item from **NanoExplorer**'s File menu.

(a) Follow steps (a) and (b) from the previous case entitled: Using the Save Sample to file... menu item ...

(b) Select File from the **NanoExplorer** menu bar, choose Export as DENEB XYZ file



(c) A new dialog appears to let you choose the file name where the sample is going to be saved in **DENEB**'s **XYZ** format. Choose the file name by mouse actions or type a new name. Click "Save".



(d) This completes the process, you can **verify** that the sample has been correctly saved in that particular file by reloading into **NanoExplorer** into a different group to avoid confusion. But note that there would not be name collisions as ***NanoExplorer*** *admits name redundancy*, it is up to the user to choose wisely the labels for the samples.

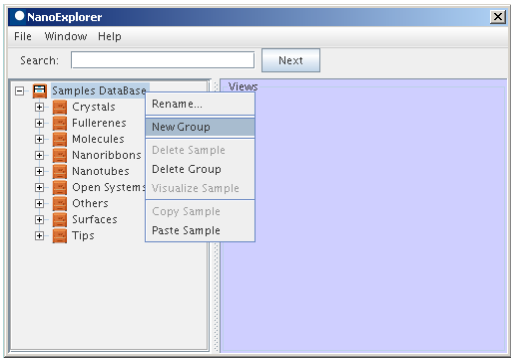
Note: If you are using **DENEB Trial** version, a maximum of 20 atoms will be exported using the XYZ format, or any format other than **DENEB**'s native.

DENEB's NanoExplorer: Organizing your samples

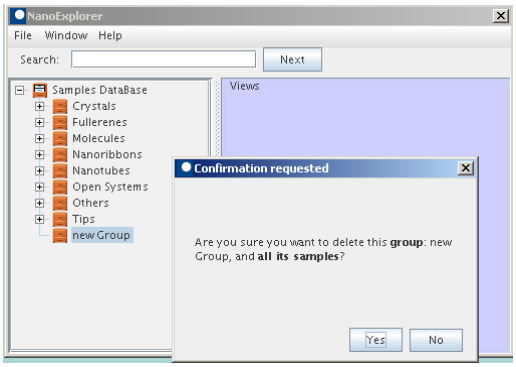
As we have said in previous sections, for DENEB, the **sample** is the basic unit that specifies a physical system. DENEB's **NanoExplorer** is a database of samples, that may contain any number of samples organized in groups in an arbitrary tree structure. The samples in **NanoExplorer** can be used as the starting point, or building blocks to compose new samples using **Sample Manipulator**. Likewise, any new sample built in **Sample Manipulator** can be stored for later use in **NanoExplorer**. The connection point among these utilities and the **Project Browser** is, as you already know, DENEB's **Clipboard**. Out of the box **NanoExplorer** comes filled out with some samples in some default tree structure, importantly, note that these are just some examples on how you can organize your **NanoExplorer** database, they are not meant to be accurate or useful for any particular purpose. **NanoExplorer** is instead intended to be your private set of own tested samples.

We show next how to **organize** the samples stored in **NanoExplorer** in a tree structure with arbitrary depth. The main operations that you need to know are the following.

1) How to create **groups** (in **NanoExplorer**, **groups** are to `samples` as folders are to files in your operating system). To create a new group in **NanoExplorer** highlight the target group, where the new group is going to be created and trigger its context menu (using `Right+Click`), select then the New Group menu item. As a consequence a new group is created with a default name, rename it if you wish using its context menu.



2) How to eliminate **groups** from the **NanoExplorer**. Select the group that is going to be eliminated and use its context menu item called Delete Group. A confirmation dialog will appear, press "Yes" to proceed with the deletion.

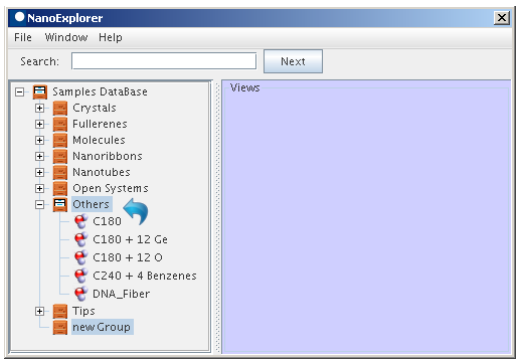


Notes:

- The deletion of a given group will eliminate all its contents (descendants).
- There is *no undo* after deletion, use therefore with care.

3) How to move a **group** (source group) into another **group** (target group) of the **NanoExplorer**. Highlight the group that you want to move, `Left-Click` and drag it, you will see that the cursor changes to the following:

This means that a drag-and-drop operation is being carried out. During the drag, the source group remains highlighted, while the possible targets will be highlighted as the cursor touches them.



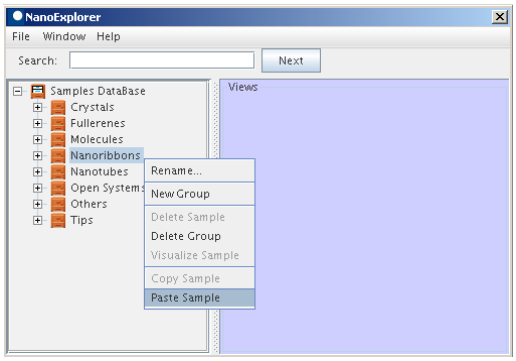
Note that only **groups** (and not **samples**) are highlighted as possible targets during the drag operation. When you reach the desired target group, release the `Left-Click`, this will complete the drag-and-drop operation. As a result the source group will be moved to become a new child of the target.

Notes:

- Before starting the drag-and-drop operation, make sure that the target group is reachable, in other words, that its ascendants are not collapsed.
- If the target group is reachable but not visible (out of the current window limits), worry not, **NanoExplorer** will automatically scroll properly while you drag.
- If the drop action is done over a **sample** (instead of a **group**), the operation will have no effect.
- If, during the drag, the cursor is taken beyond the limits of the **NanoExplorer** window, it recovers its default shape, but note that the drop action can still occur. When you "drop" out of NanoExplorer, it will still set the target at the "current row" which is deduced by extrapolation beyond its current viewport.

4) How to add **samples** to a **group**. There are two possibilities to do this:

(a) **Pasting** the **sample** stored in DENEB's **Clipboard**. To do this simply highlight the **group** where you want the **sample** to be pasted and trigger its context menu (`Right-Click`). Choose the menu item called Paste Sample.



Note:

- An exact copy of the **sample** in DENEB's **Clipboard** is added to the highlighted group. The **Clipboard** therefore maintains its contents intact.

(a) **Importing** some **sample** stored in files. Refer to the previous section about Loading samples into **NanoExplorer.**

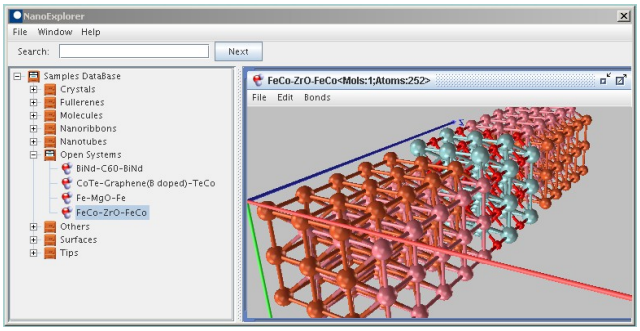
2) How to **move** a sample **from one group to another**. You can simply use the drag-and-drop technique as explained in point (3) above, only that the source is a sample instead of a group in this case.

DENEB's NanoExplorer: Backup and restore

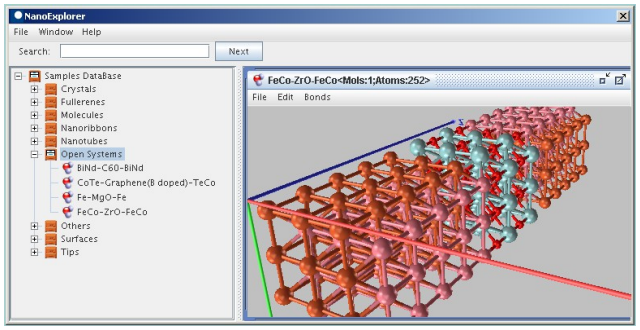
Using **DENEB**'s **NanoExplorer** you can easily export a backup-copy of any of its groups (folders) to be later on restored, possibly in a different **DENEB** installation. Note that this is compatible between systems: For example, you can backup from a **DENEB** for Windows and restore in a **DENEB** for Linux.

Here is an step by step procedure on how to backup a group:

1) Make **NanoExplorer** visible by choosing Modules → NanoExplorer or the toolbar shortcut button in **DENEB**'s main window.



2) Highlight the group that you are going to backup into a file.



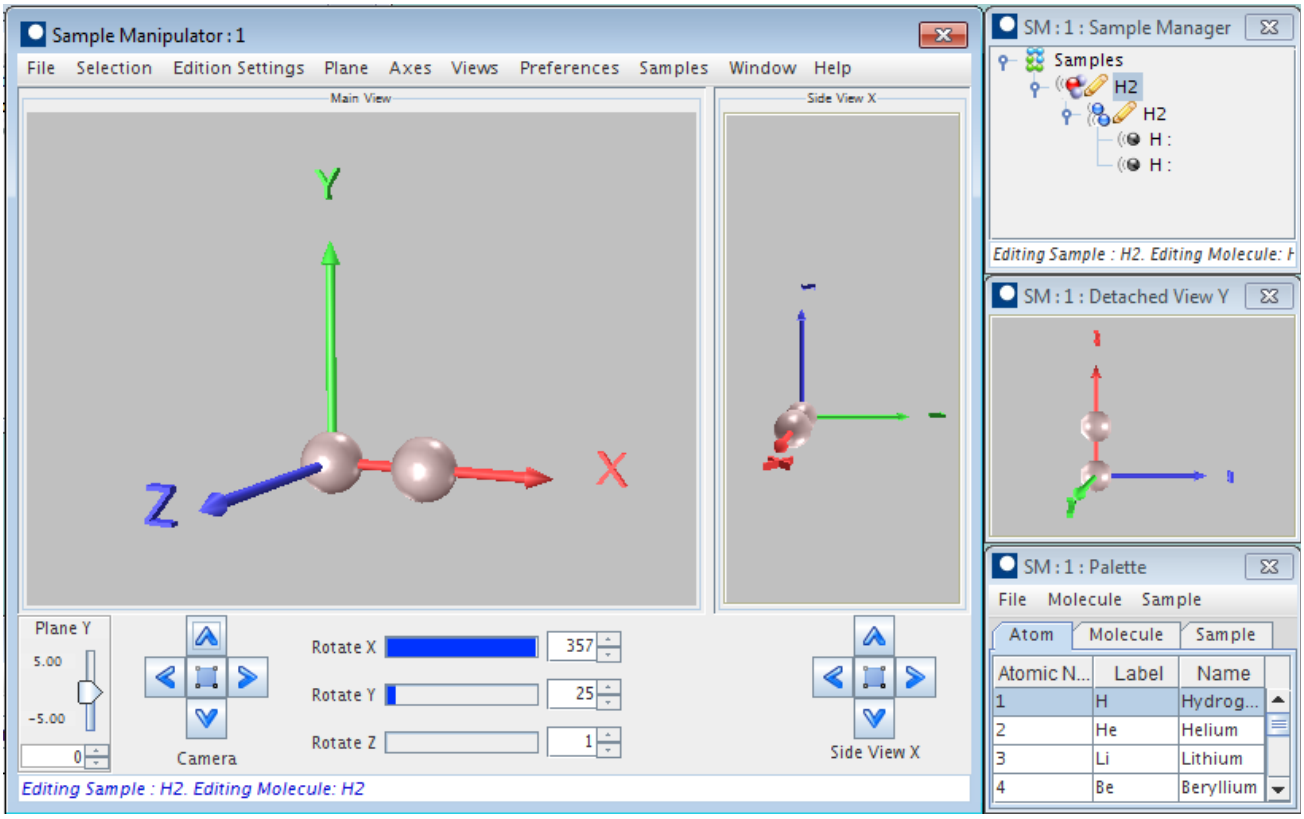
3) Choose Backup group from the File menu
4) Write the file path and file name where to save the group.
5) A confirmation dialog will appear reporting of the successful save.

And here is an step by step procedure on how to restore the saved group:

1) Highlight the group under which the restore is going to be placed.
2) Choose Restore group from the File menu.
3) Locate the desired file using the file dialog that appears and press Open.
4) The restored group will appear under the highlighted group, it is a verbatim copy of the group you saved in such file.

This ends this section about **DENEB'S NanoExplorer**.

DENEB's Sample Manipulator



DENEB Sample Manipulator: The coordinates of your objects. Absolute, local, and scaled coordinates

DENEB's **Sample Manipulator** defines a fixed, absolute Cartesian system of coordinates. Samples are placed at points with absolute coordinates.

Meaning of "placing a sample at a point": Note that a sample is an extended object, so placing it at a given point in space has to be properly defined. We properly define placing of a sample by referring to *an specific point* related to the sample, we call it the **sample's reference point**. Thus, when you place sample at a given point of space (e.g. by mouse selecting it), what you are placing there is the **sample's reference point**.

What is the sample's reference point? In DENEB's conventions, the reference point of a sample is an arbitrary point. It does not need to be its geometrical center, or the position of any of its atoms. It is the point where the **sample's local reference system** is placed. Of course, the sample's local reference system is a Cartesian coordinate system that the sample carries with it, such that all molecules that belong to that sample are placed at *local points* defined with respect to the sample's local reference system. As a consequence, if you move the sample's reference point, from an absolute point to another, all its molecules (preserving their local coordinates) move along.

Note that a molecule is to its atoms, like a sample is to its molecules. Therefore the position of an atom with respect to the molecule's local reference system is also to be properly defined. And DENEB defines it in a completely analogous way:

Meaning of "placing a molecule at a point": We properly define placing of a molecule by referring to *an specific point* related to the molecule, we call it the **molecule's reference point**. Thus, when you place a molecule at a given point, what you are placing there is the **molecule's reference point**.

What is the molecule's reference point? In DENEB's conventions, the reference point of a molecule is an arbitrary point. It does not need to be its geometrical center, or the position of any of its atoms. It is the point where the **molecule's local reference system** is placed. The molecule's local reference system is a Cartesian coordinate system that the molecule carries with it, such that all atoms that belong to that molecule are placed at *local points* defined with respect to the molecule's local reference system. As a consequence, if you move the molecule's reference point, from a point to another, all its atoms (preserving their local coordinates) move along.

Of course, at a given time, each atom is ultimately placed at a given point of space that has its absolute coordinates values. DENEB's **Sample Manipulator does present to you both the local and absolute coordinates of atoms and allows you to edit one or another at your will, keeping their synchronization at all times** (use for this the **Atom Editor** triggered by: Selection → Selection operation → Edit current selection).

In DENEB, *all reference systems have the same orientation at all times*, this is: All local or absolute, X axes are parallel to each other, and likewise about the Y and Z axes.

In Figure 1 you can see some schematic representation of the coordinate systems considered by **Sample Manipulator**.

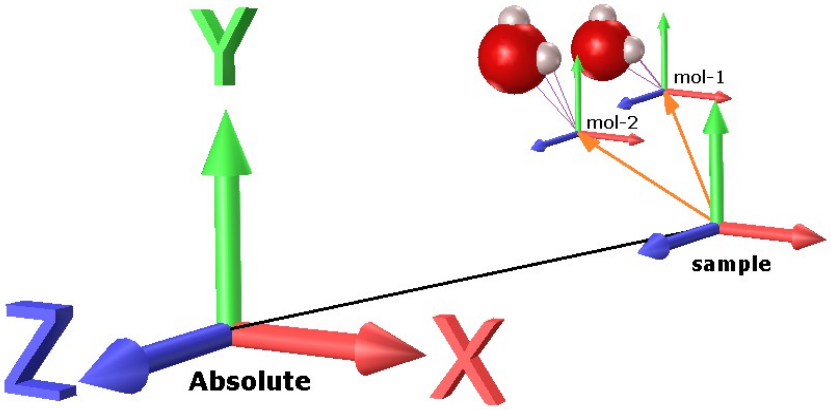


Figure1: DENEB's **Sample Manipulator coordinate systems**. A sample, consisting of two water molecules, is represented along with an skematic view of the coordinate systems considered by **Sample Manipulator.** There is an **absolute reference system** (thicker axes labeled "Absolute"), with respect to which the sample has been placed at a given point in space (the **sample's reference point**), where the axes labeled as "sample" are found. A solid black line represents the vector from the absolute origin to the sample's position. Both molecules have positions defined in local coordinates with respect to the sample's reference system. The positions of the molecules in the sample's reference system are represented by the solid orange vectors. The **molecule's local reference systems** (labeled as "mol-1" and "mol-2") are the ones with respect to which the **atom´s local coordinates** are defined. Purple thin lines represent the positions of the atoms in their molecule local systems.

Scaled coordinates: *All samples posses a so called* ***unit cell*** (a box intended for periodic repetitions). By default the unit cell is not shown, which means that the sample is 'non-periodic' (also called 'isolated'), but the user can choose to show the unit cell (using the molecule's **Sample Manager** context menu), which automatically means that the sample becomes 'periodic'. The periodic or isolated character is mostly relevant when a simulation is launched to a given engine. The unit cell box is, in turn, defined by **3 lattice vectors**, that form as well a reference system. It is usual to give the atomic coordinates with respect to the unit cell lattice vectors, in some cases it is simpler to do it this way. **Sample Manipulator** presents, as well, the **scaled coordinates** of the atoms at user's will, and allows to directly edit them, keeping perfect synchronization with respect to their local and absolute ones. To visualize/modify the scaled coordinates of any given group of atoms use the Sample Manipulator's **Atom Editor** that can be triggered from the Selection menu: Selection → Selection Operations → Edit current selection.

DENEB's Sample Manipulator: Translating and rotating objects

Meaning of translating samples, molecules and atoms: in **Sample Manipulator** you will learn that you can translate atoms, molecules and samples. What is the difference between 'moving all atoms in a molecule' and 'moving the molecule itself'? If you select all atoms in a molecule and shift their position by a vector (using the main menu option: Selection → Selection Operations → Translate, that applies to atoms) you are changing their local coordinates with respect to their local reference system (with respect to their molecule's reference system). However, if you choose to shift the position of the molecule itself (using that molecule's context menu in the **Sample Manager**) you are keeping fixed the local coordinates of the atoms but you are changing the coordinates of the molecule with respect to its sample's local reference system. Visually, however, you will see the atoms displacing just in the same way. Likewise, it is not the same to translate all molecules in a sample than to translate the sample itself. A bit of practice will surely let you learn these simple concepts readily.

Meaning of rotating samples, molecules and atoms: in **Sample Manipulator** you will learn that you can rotate atoms, molecules and samples with respect to arbitrary axes. What is the difference between 'rotating all atoms in a molecule' and 'rotating the molecule itself'? If you select all atoms in a molecule and rotate their position by an angle with respect to a given axis (using the main menu option: Selection → Selection operations → Rotation, that applies to all selected atoms), you are changing their local coordinates with respect to their local reference system (molecule's reference system). However, if you choose to rotate the position of the molecule itself (using the **Sample Manager** context menu of that molecule), you are keeping fixed the local coordinates of the atoms and you are just displacing (around the rotation axis) the molecule's reference point, whose local coordinates (with respect to its sample's local reference system) will change. In fact, unlike in the translation case, these two cases result in really different atomic motions: For example if the molecule's reference point lays on the rotation axis, the "rotations of the molecule" leave everything unchanged; while it is not so if one chooses to rotate the atoms individually.
Likewise, it is not the same to 'rotate all molecules in a sample' than 'to rotate the sample itself' (which just displaces its reference point). A bit of practice with **Sample Manipulator** will surely help you learn these concepts better, as well.

DENEB's Sample Manipulator: The plane.

To edit your samples use DENEB's **Sample Manipulator**. This tool provides with extensive abilities to build samples from scratch, combine them into new ones, and modify existing ones. With **Sample Manipulator** you have complete freedom to edit your samples in almost any imaginable way. It introduces new concepts and auxiliary graphical tools that enable accurate manipulation and navigation. The **Plane** of the **Sample Manipulator** is one of such tools. It is an auxiliary object that helps in several ways:

- Enables accurate mouse-picking of points in the three dimensional space, for several uses: for placement of new objects, placement of center of rotation of the main view camera, displaying the coordinates of an specific mouse-picked point.
- Provides a geometrical reference to select/un-select atoms according to their position. (Note that one can also select/un-select atoms in other ways: By mouse picking `Ctrl+LeftClick` (selects an atom, molecule, or sample depending on the mode), by context menus of the items in **Sample Manager**, by context menus of **Atom Editor**).

The **Plane** is just that: An infinite plane that can be placed perpendicular either to X, Y, or the Z axis and at any height within. Its orientation can be controlled with Plane → Plane settings → Perpendicular to, and its position can be controlled with the **plane control-panel** placed at the bottom-left corner of the **Sample Manipulator**'s main window. The **plane control-panel** is a combined slider, text, and spinner-buttons synchronized input system, you can specify the plane's position by either of them. The plane's motion range can be modified by Plane → Plane settings → Set motion range, that has the key short-cut `Ctrl+R`.
Even though the plane is infinite, its visual representation is rather not, so we can actually see it better.

Its representation is a rectangular area of a user chosen size, position (within the plane) and color. To choose these **visual settings of the plane** use: Plane → Visual → Select color, and Plane → Visual → Select visible size, respectively.

> **Hint:** the plane can be also used as a location template by simply playing with its variable visual shape and size, e.g, if you wish to place 4 atoms in an square configuration of a given size you can simply choose the plane to have that shape and size, and then `Click-place` the atoms at its vertices.

DENEB's Sample Manipulator: Simple building

There are many different ways to construct new samples using Sample Manipulator. In general you will probably start with some already made samples, modify them and/or combine them into new ones. Nevertheless, for the sake of simplicity, we describe here the case in which you start with a clean slate:

1) **How to build a simple molecule from scratch:**
   a) From DENEB's main menu bar choose: Modules → Sample Manipulator → New. This will create and show a new **Sample Manipulator**. A toolbar short-cut button for this menu item can be also found just below the main menu bar. This is how it looks:

The main larger button creates a new **Sample Manipulator** when pressed, while the smaller button at its right gives short-cut access to the already created Sample Manipulators (if any).

   b) From the newly created **Sample Manipulator**, choose the tab "sample" in the **Palette** window, placed by default at the bottom right. Select the sample called "Empty", it is a sample with one empty molecule, where we can add atoms to fill it up at will.
   c) To place the Empty sample in space `Left-Click` at some point of the **Main's View Plane**. By default the plane is seen as a yellow square of 5 Angs of size. Since it is empty, in this case, you will notice that a new sample has been created not because of the appearance of atoms (spheres) at the scene, but because of the appearance of a new branch in the **Sample Manager** window (placed at the upper left corner of the **Sample Manipulator** by default).
   d) Rename the sample. To do it, highlight its name in the **Sample Manager** and `Right-Click` on it to trigger its context menu. Choose Rename this sample. Likewise do the same with its molecule that has no name by default. We have chosen "H2" as names for this example.

   e) Now set the molecule and sample that are going to be edited, in this case, the only molecule and sample that there are in the scene. To this aim, highlight the sample "H2" in the **Sample Manager** and `Right-Click` on it to trigger its context menu. Select Set as sample being edited. Its icon changes after this selection, a pencil is added as symbol of being edited. This setting is necessary so the Sample Manipulator knows what sample is the one that is receiving the new molecules that we may add by clicking on the scene. Likewise select the molecule and trigger its context menu, select Set as molecule being edited. This settings is necessary so the Sample Manipulator knows what molecule is the one that is receiving the new atoms that we may add by clicking on the scene.

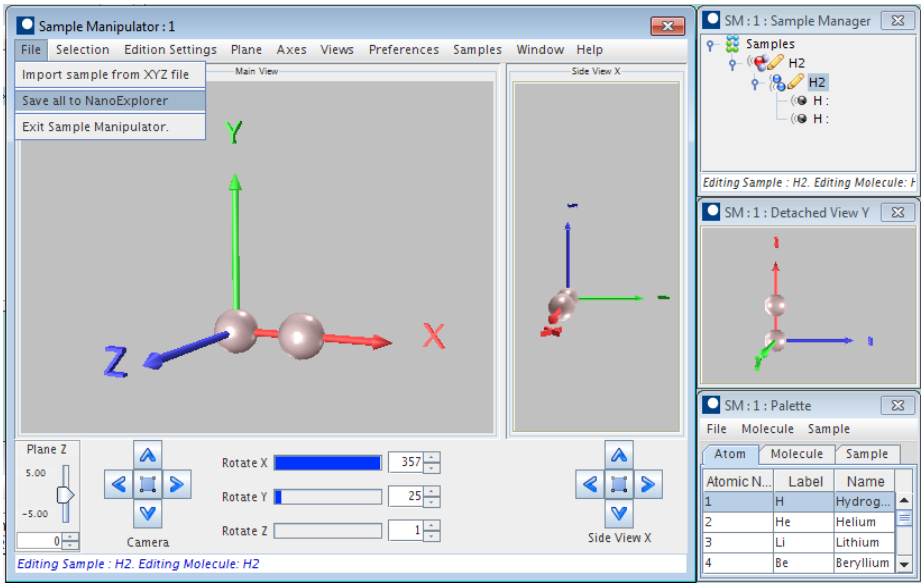
   f) Now lets add a couple of atoms to the molecule being edited. To this aim, select the Atom tab in the **Palette** and highlight the Hydrogen atom on the list. `Left-Click` on the plane at couple of positions to produce a couple of new atoms. *Hint*: if you wish to delete some atom use `Shift + Left-Click` on it. Now lets select them, to do this, simply `Ctrl + Left-Click` on them. Once selected we can trigger the **Atom Editor** to accurately edit their positions. Use Selection → Selection operations → Edit current selection

   g) Lets use the **Atom Editor** to set their local-coordinates to (0,0,0) and (1,0,0) respectively. These are the coordinates at their molecule's reference system. To do this, you will have to display their local-coordinates by selecting Local from the context menu Coordinates → Local.

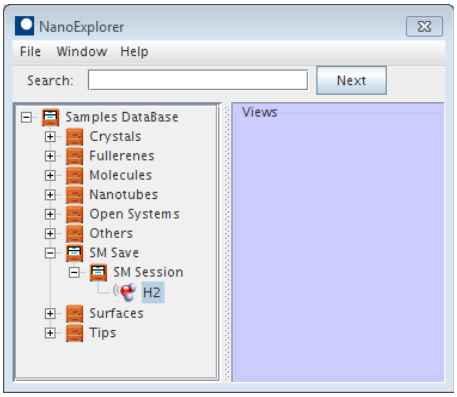
h) You can simply type-in the new local coordinates.

i) Finally place the sample's reference point at the origin (0,0,0) by using Move → Place this sample at a point, from its context menu at the **Sample Manager** tree. Likewise place the molecule's reference point at the origin using its context menu.

j) To give persistence to your newly created sample there are several ways, for example you can select Save all to NanoExplorer from the File menu in the **Sample Manipulator**,

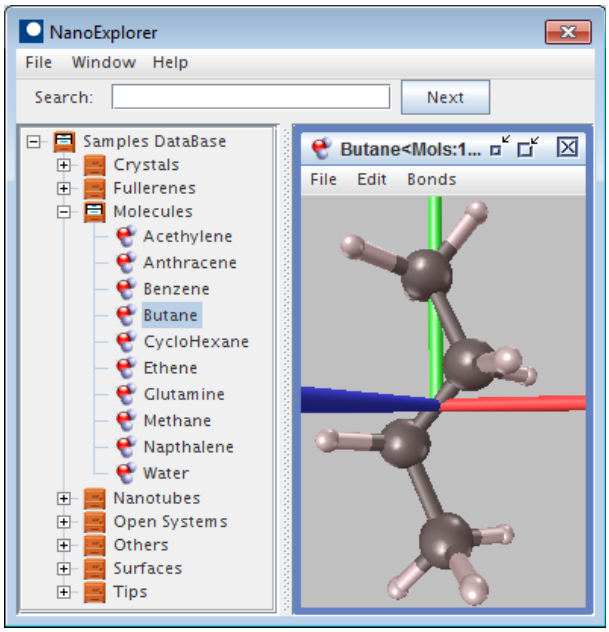


choose a name for the folder that will hold the sample in **NanoExplorer**, or accept the default name "`SM Session`", in such case the resulting path for our sample in the NanoExplorer database will be: `SM Save → SM Session → H2`



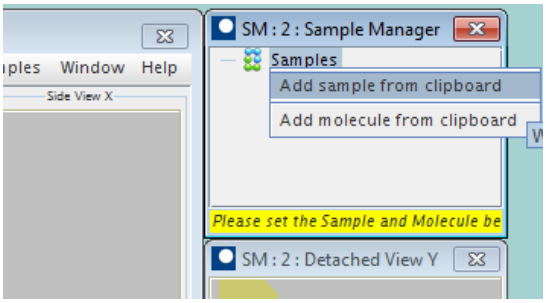
2) How to modify an already built sample:

a) Let us modify a sample by simply stretching one of its bonds. Let us choose the sample called `Butane`, find it in **NanoExplorer,** under the folder group called `Molecules`:

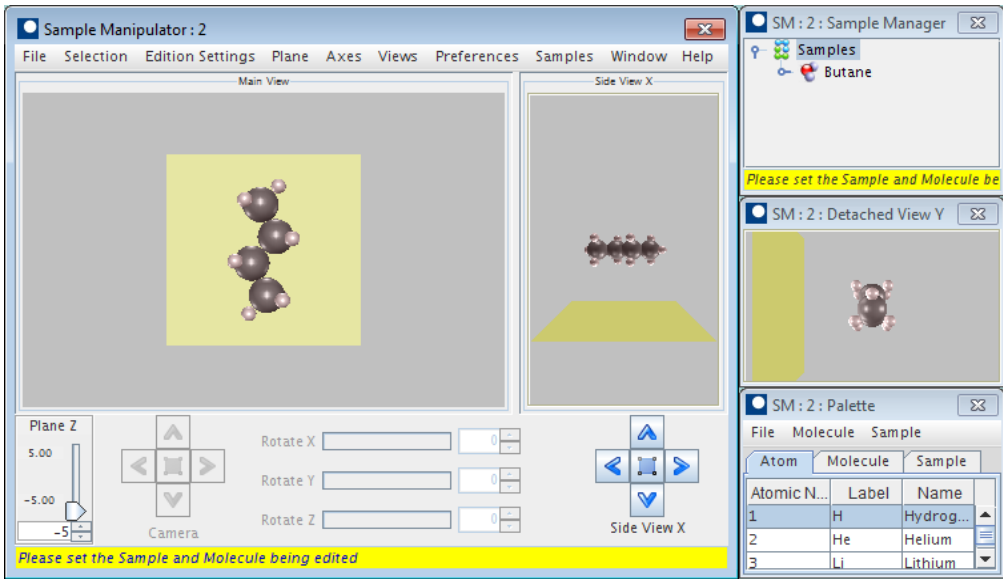


b) Choose Edit → Copy to clipboard from the samples visualization window menu or Copy Sample from its context menu in the tree representation. This places an identical copy of the sample in DENEB's **Clipboard**.

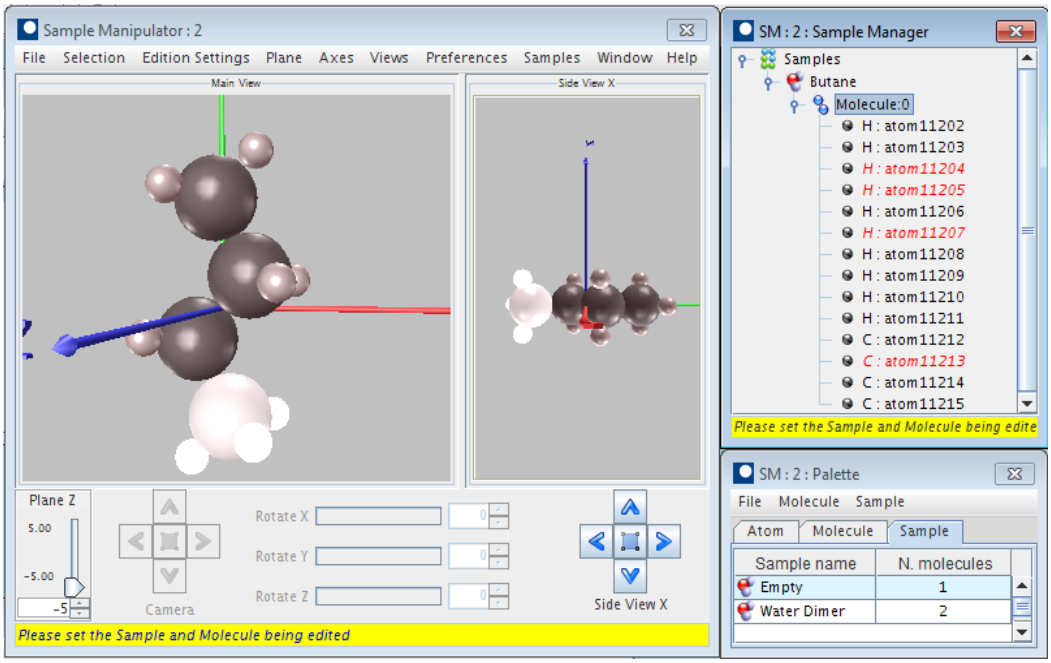
c) Open a new Sample Manipulator and paste the Clipboard contents (in this case the copy of the sample called Butane) in it. To do this, choose Add sample from clipboard from the context menu at the root of the **Samples Manager**:



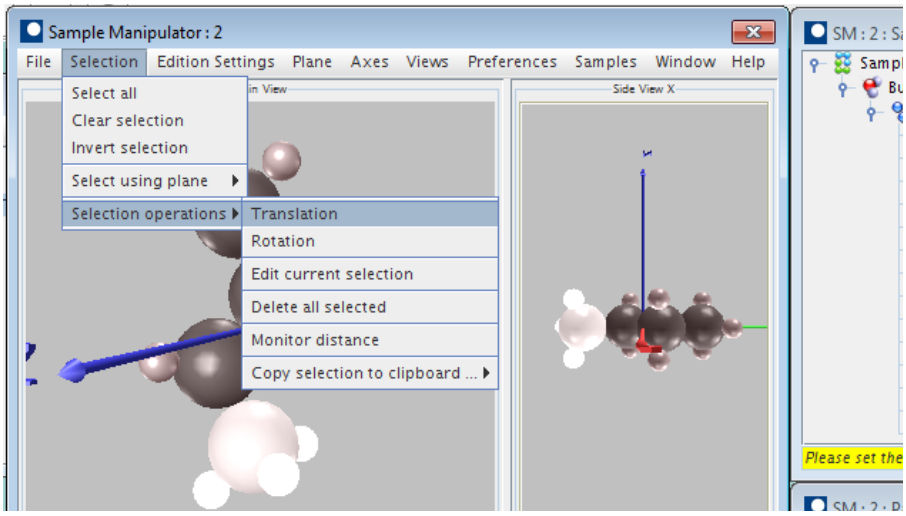
The result is that a copy of the sample called Butane is placed in the sample manipulator, its reference point at (0,0,0):



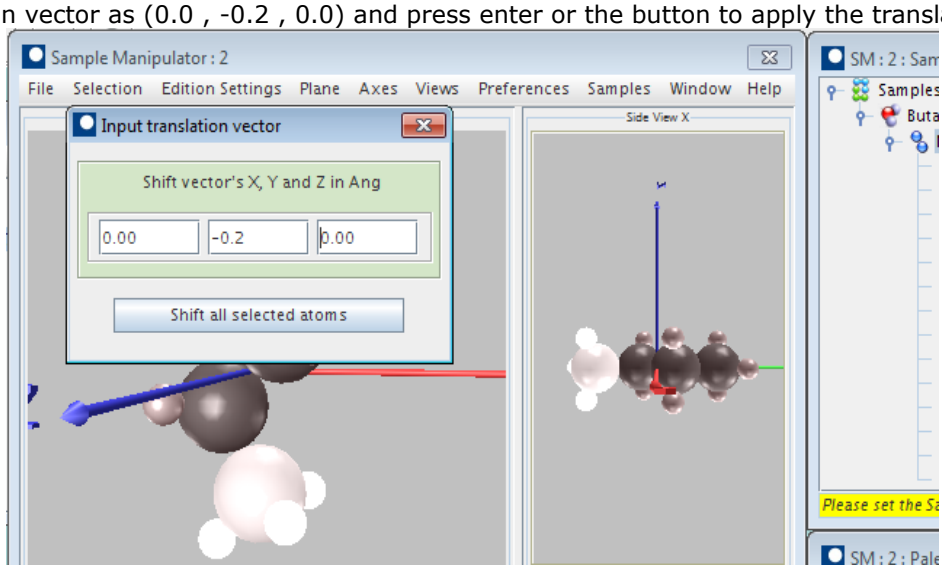
d) Press `Ctrl + Left-Click` on the C atom at the lower extreme (along Y), and on its three Hydrogen neighbors. The result should be that they are selected, and thereby "glowing" with respect to the rest. On the **Sample Manager**, the selected atoms appear in red ink and in italics.



e) We are going to displace the four selected atoms 0.2 Ang along Y, this will stretch the C-C bond. To this aim, choose Selection → Selection operations → Translation from the **Sample Manipulator** main menu.

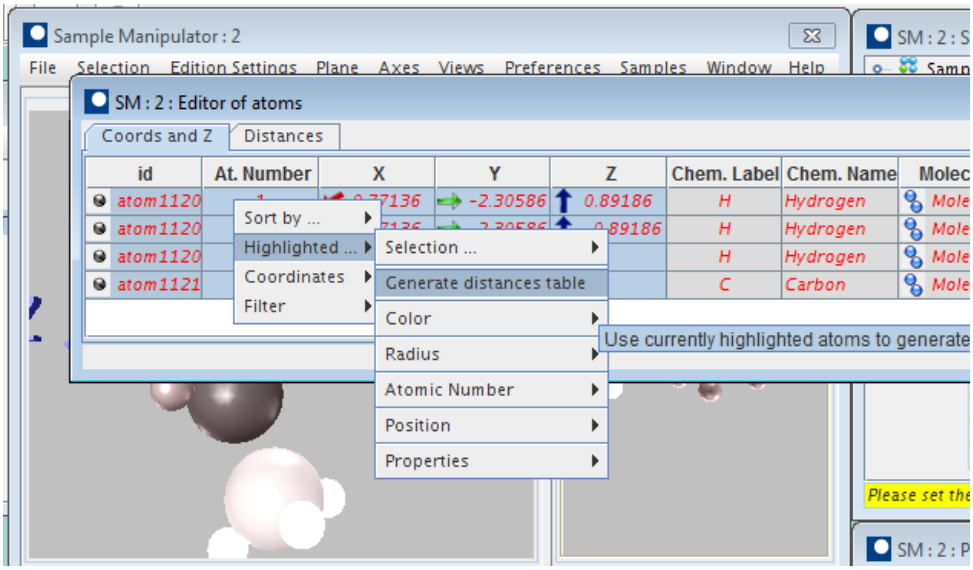


Set the translation vector as (0.0 , -0.2 , 0.0) and press enter or the button to apply the translation.



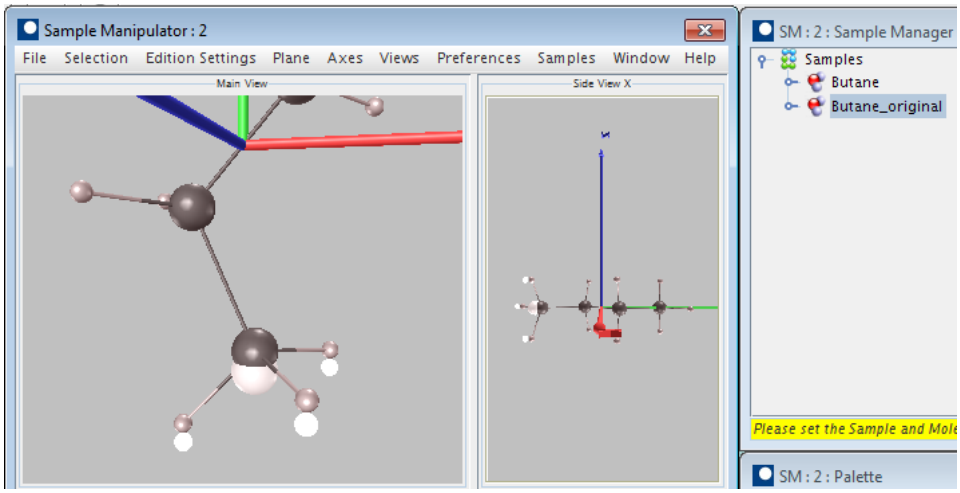
f) Note: to monitor how the distance between two atoms changes in real time, you can use the Selection → Selection operations → Monitor distance tool.

You can also measure the distances between atoms by using the **Distances** tab of the **Atom Editor**, which is filled out when Generate distances table is chosen from the context menu in the same Atom Editor, at the option: Highlighted → Generate distances table. This fills the **Distances** tab with a table of distances for the currently highlighted atoms in the Atom Editor's list.



Note: Do not confuse the *highlighted* atoms in the **Atom Editor** with the (glowing) *selected* atoms in space, they might refer to the same atoms, but they need not. We reserve the word "*selected*" for the glowing atoms, the "Selection" menu applies to them. However the word "highlighted" is used for those rows highlighted at the **Atom Editor** or those branches highlighted at the **Sample Manager**, whose corresponding atom might or might be not selected (glowing). Incidentally, note that operations on the selected (glowing) atoms are grouped under the menu called Selection, while operations on molecules and samples as a whole are grouped at the **Sample Manager** tree context menus.

g) To visually compare the new stretched sample with the original one is simple, we can just paste again a second copy of the original one and see the superimposed representations.



Note: To obtain the previous snapshot, we have:

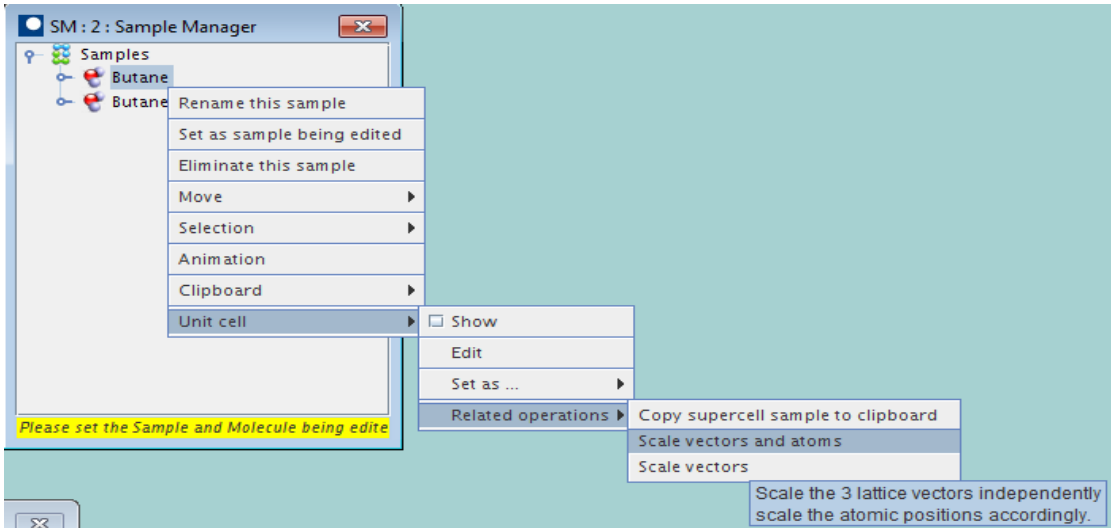
- pasted again the same sample (Butane) and renamed it as Butane_original,
- then reduced all atoms radii as follows: Selected all atoms, then triggered the **Atom Editor** for them by Selection → Selection operations → Edit current selection; then highlighted all rows; then used the Atom Editor's context menu Highlighted → Radius → Edit radius.
- Then we have cleared the selection (Selection → Clear), and re-selected only the atoms of Butane_original (using its context menu in the tree of **Sample Manager**).
- Finally, we used Preferences → Bonds ... → Re-calculate bonds → Between selected atoms to show bonds between the atoms of Butane_original. Where we had chosen `0.02 Ang` for the bond radii at the bonds settings menu.

DENEB's Sample Manipulator: Building Periodic samples

Difference between periodic and non-periodic samples

All samples in **DENEB** have a so-called **Unit-Cell**. Even though you might have not defined any, all samples have a unit cell which is set as a cube of one Ang size by default. So what is the difference between a periodic sample and a non-periodic one? Periodic samples are those whose Unit-cell is being shown. To make the Unit-cell show, simply select the check-box Show from the sample's context menu: Unit cell → Show, so you make it periodic. Conversely un-select the check-box Show to render the sample non-periodic. If a unit cell of a sample is "hidden", that fact does not erase in any way its parameters, you can even modify and edit the unit cell parameters while it is being hidden. You can modify a sample's unit cell by using its context menu options:

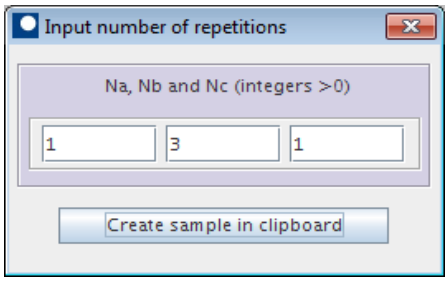
- Unit cell → Edit
- Unit cell → Set as ... ;
- Unit cell → Scale vectors;
- Unit cell → Scale vectors and atoms



Therefore, if you want the unit cell to be taken into account when its sample's corresponding **Job** is launched, make sure that the Unit-cell is "showing" when you copy-paste the sample into a **simulation** (simulations are found at the **Project Browser**). Note that some calculation engines have the option of specifying or not a unit cell, so this would correspond to showing or not the unit cell in **DENEB**.

The unit cell as a building tool

Note that a periodic sample usually represents an infinitely extended system that covers the whole 3D space. However, in **DENEB** the only atoms that are shown, are those of the unit cell. Therefore, sometimes you might need to plot not only the unit cell but some repetitions of it, in order to visualize better the extended system. To do so you can simply create a **supercell sample** from the original one. This new sample is simply made by integer repetitions of the unit cell along its lattice vectors. To this aim, use: Unit cell → Related operations → Copy supercell sample to clipboard. You will be asked the number of repetitions of the unit cell along each vector, and a new sample will be made using those parameters, its corresponding unit cell will be as well resized exactly along.

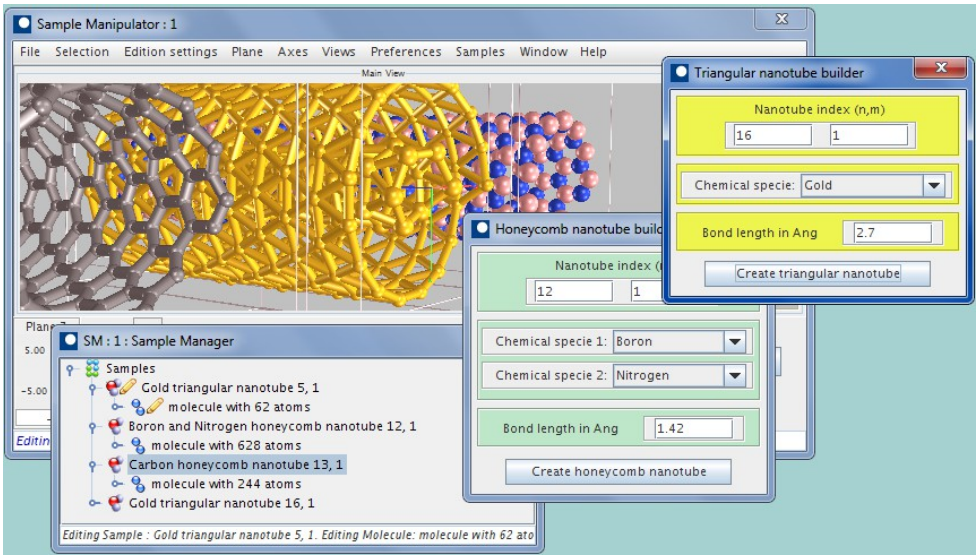


The new sample is placed in DENEB's **Clipboard**, so you can paste it back where you wish (Sample Manipulator's **Sample Manager**, Sample Manipulator's **Palette**, **NanoExplorer**, **Project Browser**). You can use the Copy supercell sample to clipboard, menu item to quickly produce parts of samples that keep some periodicity, it is simple to produce for example, surface slabs, nanowires, etc.

DENEB's Sample Manipulator: Nanotube Builders

From DENEB 1.26, **Sample Manipulator** includes nanotube builders; find them under the menu Samples → Builders. The different kind of nanotube builders are labeled according to the corresponding two-dimensional lattice. Thus, out of the box, DENEB 1.26 comes with **honey-comb** and **triangular** nanotube builders. Its use is very simple: Just press the button "Create nanotube …". Of course, if you want to build nanotubes different from the default you have to modify their parameters, which are:

- The chemical species of the atom/s of the 2D unit-cell basis.
- The nanotube chiral vector indices, typically called (n,m).
- The first-neighbors bond-length in the 2D lattice. (Note: interatomic distances might slightly change once the 2D sheet is wrapped around to produce the nanotube)



Upon pressing the "create" button, a nanotube is produced (as a new sample) and added to the **Sample Manipulator** at the origin. The builders algorithm also produces its unit-cell; it is accurately computed such that supercell repetitions along the tube's axis do perfectly match. In turn, the perpendicular lattice vectors are chosen a bit arbitrarily to form a sufficiently large square; you can easily modify these lattice vectors -as you know- using the samples context menu at the **Sample Manager**.

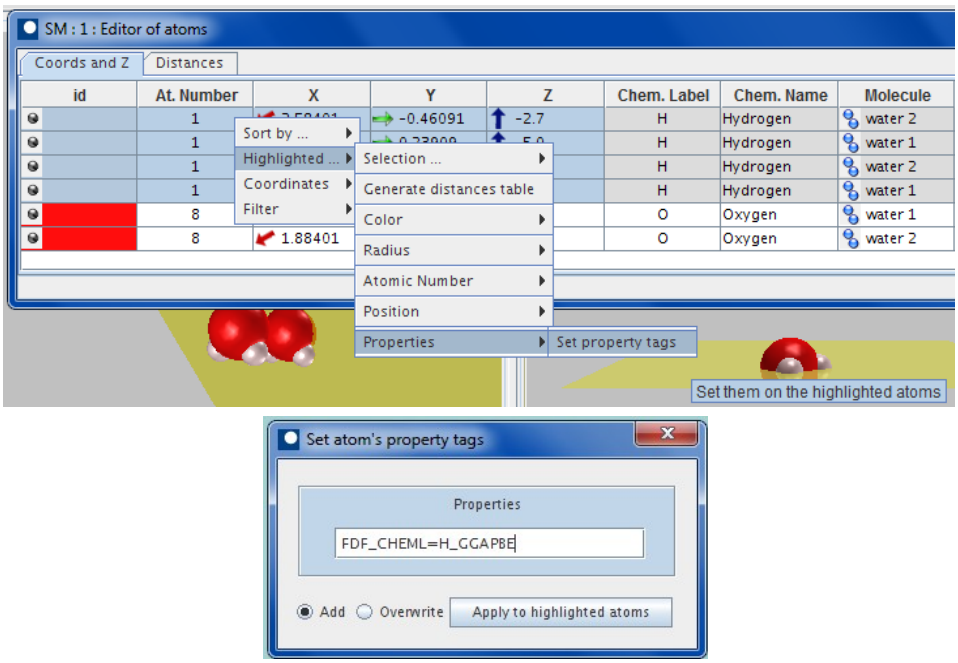
DENEB's Sample Manipulator: Using the atom "Properties"

Sometimes there are computational parameters that are attached to an specific atom. You can set these parameters in the Properties column of the **Atom Editor** in the **Sample Manipulator**. The property-tags can be multiple for any given atom, the general format that you can use to write them is the following:

`<Label1>=<Value1>;<Label2>=<Value2>;...`

This is, a semicolon-separated series of `label` and `value` pairs separated by the character "=". A syntax exception is that for boolean labels you need not to assign a value, **DENEB** understands that a boolean label is "true" when it appears, and does not parse further in search for its value.

To modify the property tags of some atom, you can directly type in the corresponding cell using the Sample Manipulator's **Atom Editor**. You can also ***massively change the property tags of many atoms*** using the Atom Editor's context menu: Highlighted → Properties → Set property tags. With this option, you can either **add** a property-tag to a given list of atoms (those highlighted), or you can entirely **overwrite** their properties string.

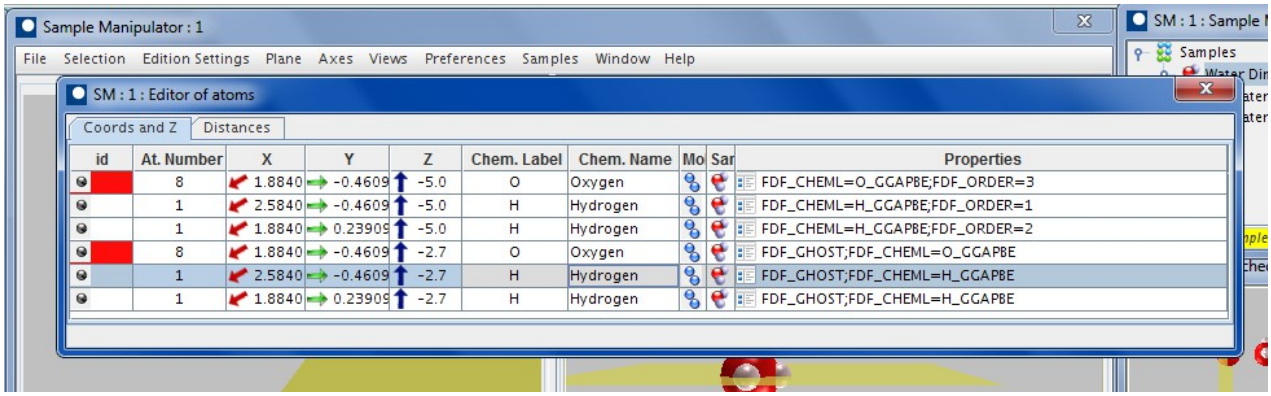


Each simulation type has its set of Property tags in **DENEB**, we list them here grouped as a function of the calculation-engine:

Property-tags for the simulations of the type SIESTA:

1. **FDF_ORDER**. Defines the order in which the atom will be written in the corresponding `.fdf` file. Example of use: `FDF_ORDER=1`. Note: **DENEB** automatically sets this property on atoms from samples that are loaded from `.fdf` files, remembering, this way, their order in such file.
2. **FDF_CHEML**. Defines the chemical species label that this atom will be assigned to in the `.fdf` file. Example of use: `FDF_CHEML=H_GGAPBE`. Note: you do not need to specify it when the chemical species label desired is the default which is equal to the chemical species symbol.
3. **FDF_GHOST**. Defines whether this atom will be considered as a ghost atom in the corresponding SIESTA simulation when executed. Do not specify a value for this variable, its presence gives the value of `true` automatically, its absence defaults to `false`. Example of use: `FDF_GHOST`.

See the following figure as an example where some property-tags are already defined for several atoms:



DENEB's Sample Manipulator: Animation of samples

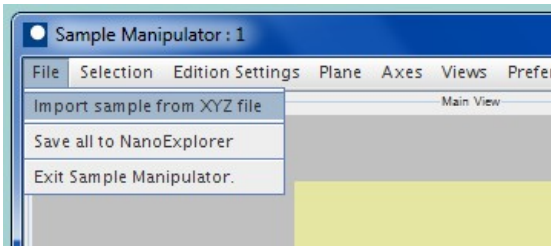
You can instruct for **Sample Manipulator** to load a file with the animation of a sample. This file should be in the **`xyz` format**. In this simple format the list of atoms is given as the chemical species symbol followed by the coordinates of the atom in Angstroms. There is a header consisting of two lines: the first line contains only the number of atoms, while the second line is an arbitrary comment that can be left blank eventually (but can not be removed). In this format one can subsequently attach one set of atoms after another in the same file. **DENEB** can load these "multi-frame files" doing the interpretation of each set **either** as a new molecule of the same sample, **or** as a new frame (*instantaneous photo* or *time step*) of the **dynamics** of a given sample. Use **Sample Manipulator** to open multi-frame `XYZ` files selecting one of these options, note that when you select to load a multi-frame `XYZ` file as the dynamics of the same set of atoms, one requisite, that **DENEB** checks for, is that all frames refer to the same set of atoms at different times, i.e. The number of atoms should coincide for all frames, and the chemical species should also coincide from one frame to the next. These conditions need not to be met when the file is loaded using the other modality: that of considering each frame as a different molecule of the same sample. A last note about the `XYZ` format as understood by **DENEB** is that one can use the comment line to instruct **DENEB** with useful information. In particular one can define the `Unit Cell` of the sample in such comment line (or the comment line corresponding to the first frame in the case of multi-frame files). To achieve this, simply write the unit cell lattice vectors in the comment line as follows:
`latticeVectors:[ ax ay az#bx by bz#cx cy cz ]` being (ax,ay,az) the coordinates of the first lattice vector ins Angs, (bx,by,bz) the coordinates of the second, and so on and so forth. This way, the so called **DENEB**'s **`xyz`** format is compatible but extends the capabilities of the standard **`xyz`** format. Here is a verbatim example of a multi-frame file in **DENEB**'s **`xyz`** format:

```
3
latticeVectors:[ 5.0 0.0 0.0 # 0.0 7.0 0.0 # 0.0 0.0 6.0 ]
O    0.0   0.0   0.0
H    0.8   0.0   0.0
H   -0.2   0.7   0.0
3

O    0.0   0.0   1.0
H    0.8   0.0   1.0
H   -0.2   0.7   1.0
3

O    0.0   0.0   2.0
H    0.8   0.0   2.0
H   -0.2   0.7   2.0
3
```

```
O    0.0   0.0   4.0
H    0.8   0.0   4.0
H   -0.2   0.7   4.0
```

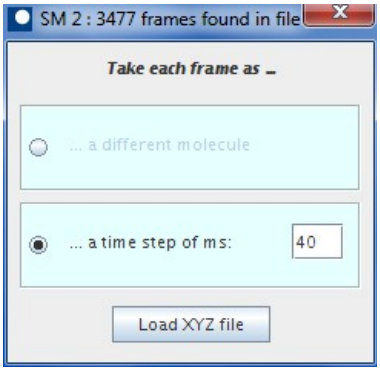
It contains four frames that represent the same set of atoms only that are displaced by one Ang along the Z axis from one frame to the next. Therefore in this case you could optionally load (using **Sample Manipulator,** see below) this file as a time series or as a series of molecules that belong to the same sample.

In the following we give specific instructions on **how to load an animation file** and how to control the animation with the sample's Animation Control Panel :



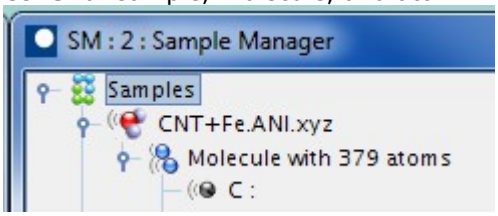
(a) Load the sample with the animation from a file. Choose File → Import from XYZ file

(b) Once chosen the file to be loaded, **Sample Manipulator** will try to load it. Wait for a little while if necessary, big files require some seconds to process. **Sample Manipulator** will detect if there is more than 1 frame. In that case it lets you choose the type of loading: (a) each frame considered as a new molecule, **or** (b) each frame considered as a time step in the evolution of the same sample.

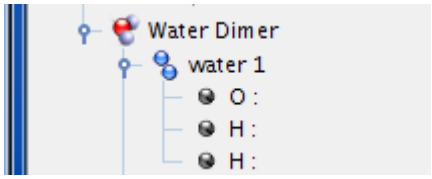


(c) Select the radial button labeled "... a time step of ms" and input the **real time** that each frame will be displayed in milliseconds (or simply accept the suggested value of 40 ms for a smooth display). Press Load XYZ File. The sample will be then loaded and displayed in **Sample Manipulator**. Notice that its corresponding icon in the Sample Manipulator's **Sample Manager**, indicates that the sample contains a trajectory:

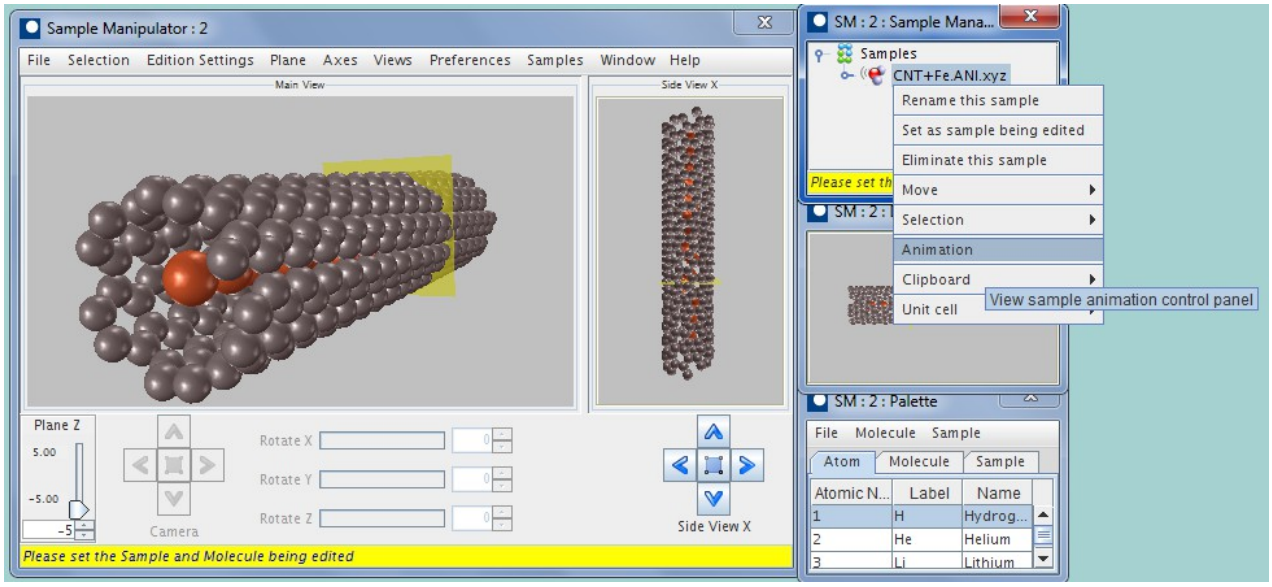
Here is an example of how the **icons** for sample, molecule, and atom **with trajectories** look:



While the corresponding **icons** for sample, molecule and atom **with no trajectory** are, as you may already know, slightly different, here is an example:

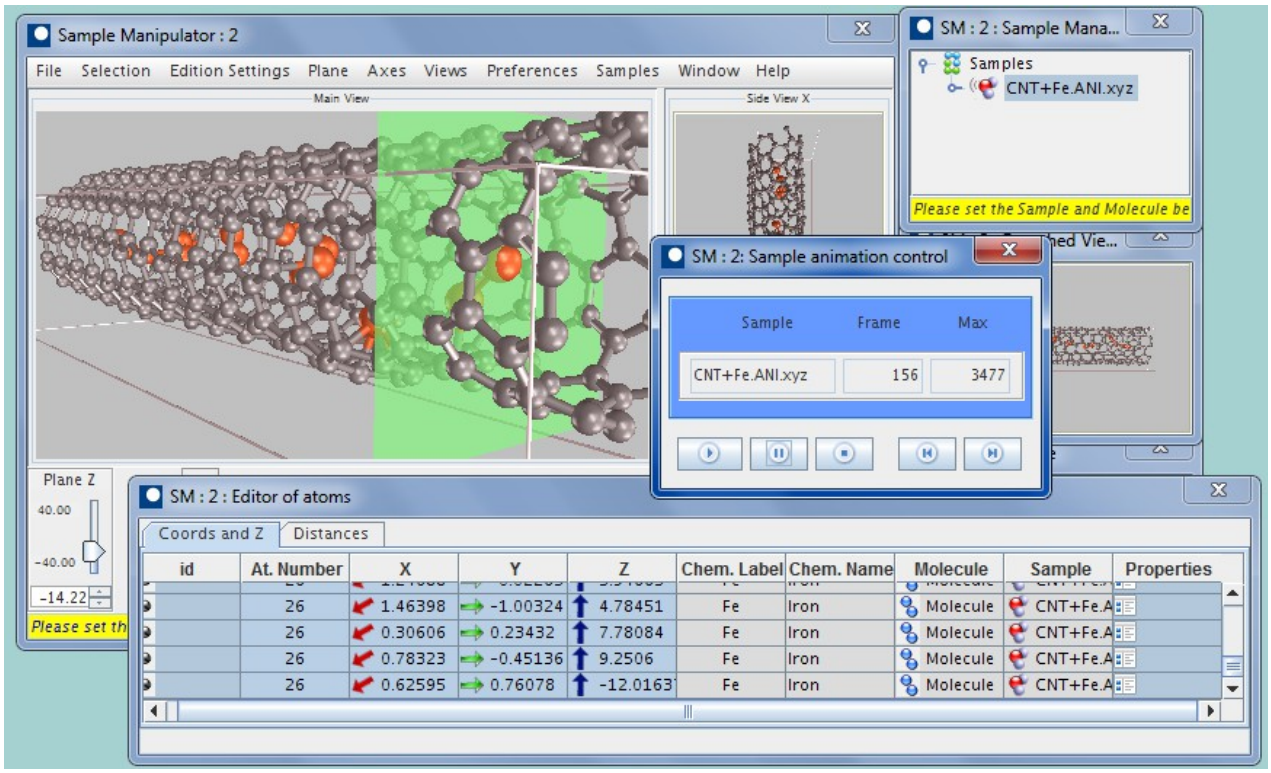


(d) To access the Animation Control Panel of the just loaded sample use its context menu called Animation.



(e) The Sample animation control dialog will appear. This panel provides controls to the animation of the sample, find in it the buttons for:

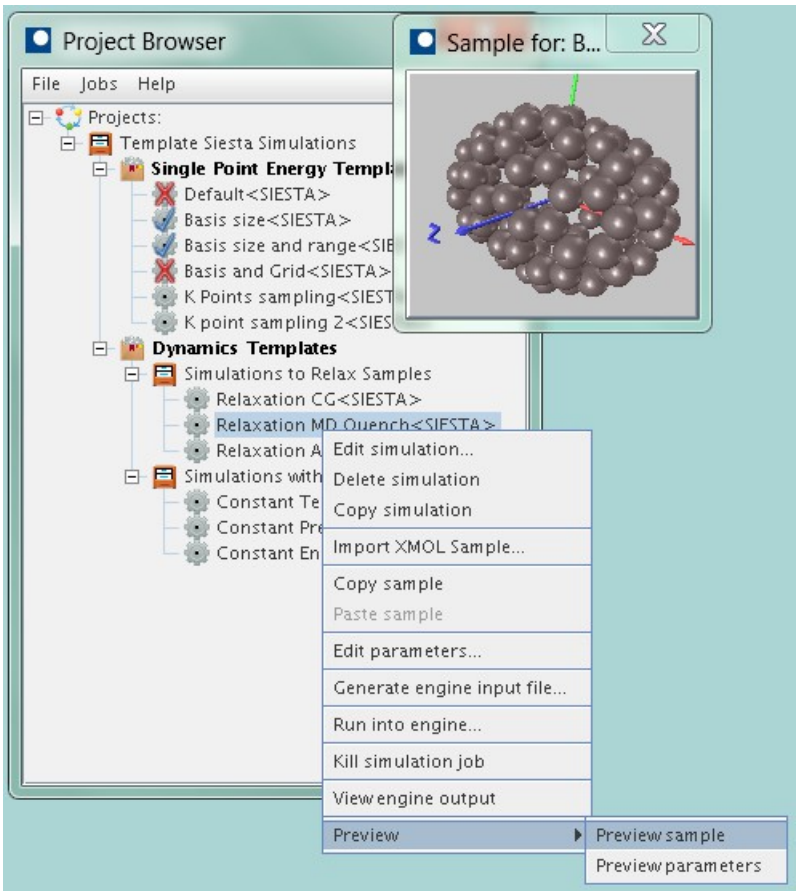
- Play
- Pause
- Reset to initial positions
- Advance one frame
- Return one frame



Notes about the animation of samples:

- Depending on the performance of your hardware, and the number of atoms in motion, the animation display could be more or less smooth.
- If bonds are showing (`Preferences → Bonds → Show`) you will notice that they do not follow the dynamics of the animation. This is a feature aimed not to hinder performance. Therefore, you will probably want to observe the dynamics while not showing bonds, and to recalculate bonds when wanted at specific frames (`Preferences → Bonds → Re-calculate bonds → …`).

DENEB's Project Browser



DENEB's Project Browser: General idea.

As we have mentioned earlier, **DENEB**'s aim is to facilitate and expedite the work of researchers in the fields of *Atomistic Simulations*. With **DENEB** you can create, execute, retrieve, organize and centralize your thousands of simulations belonging to your hundreds of research **projects**. **DENEB**'s **Project Browser** is the place where you can create, modify, organize, classify and centralize all your **projects**.

From **DENEB**'s **Project Browser**, you can create **simulations** by coupling a given **sample** to a given set of computational **parameters**. Your simulations might apply to very many different physical systems, they could also belong to different *calculation engines* (e.g. **SIESTA**, **QuantumEspresso**, **CPMD**, **VASP**, etc), and could be launched for execution into several different remote hosts … In spite of this, **Project Browser** can keep track of each of them and present them to you neatly organized and readily accessible. Using **DENEB**´s **Project Browser** you can choose any kind of classification for your simulations, based on kind of sample, type of calculation engine, etc. Use customary labels and organize them, in groups and projects, into tree structures of any depth. Quickly search and -with a single click- store/retrieve all of it: Simulations, projects, their organization, and their resulting data.

DENEB's Project Browser: The concept of project and simulation.

We have already used these words (**project** and **simulation**), but let us properly define them with regard to **DENEB**'s understanding before continuing.

Definition of project:
A **project** in **DENEB**'s terms, is loosely defined as the set of **simulations** corresponding to a given real-life research project. These can be just a few or very many; a **project** can, thereby, have an internal classification structure of any complexity, customarily defined into a tree-organization. But a project can not contain another project within.

Definition of simulation:
A **simulation** in **DENEB**'s terms, is loosely defined as a representation of a ready-to-use input-file for some calculation engine. **DENEB** considers that all **simulations** are composed of **two** distinct parts:

1. The **sample**, where the physical system is defined. Which is the object that **NanoExplorer** and **Sample Manipulator** are dedicated to.
2. The **parameters**, which are the rest of computational parameters (related to the scientific model, the numerical precision, etc) that a calculation-engine needs to completely define a single execution run. This is the object to which the **Parameters Editor** is dedicated to.

> **Note**: Some little mixing is unavoidable, for example the property-tags, that you can edit using the **Atom Editor** of **Sample Manipulator**, reflect properties of the atoms that are not strictly related to the definition of the physical system itself, but rather to the calculation according to some calculation-engine.

The **Project Browser tree**, presents different **icons** for different kind of objects, this facilitates that you quickly know what are you looking at, here is an example:

Project Browser shows all your **projects** and **simulations** in a tree structure with arbitrary depth, and lets you organize them in **groups** as you wish. **DENEB** represents these kind of objects with different icons:

-  → Icon for the **root** of this tree structure, labeled "Projects".
-  → Icon for a **group** of objects. **Project Browser** can hold as many groups as you wish, nested arbitrarily.

-  → Icon for a **project** object. **Projects** may contain any number of **groups** and **simulations,** but can not contain another **project**.
-  → Icon for a **simulation** object. A **simulation** must always belong to a **project**. They are leaves of this tree, i.e. they have no "descendant" branches. Each **simulation** necessarily belongs to a given type determined by the kind of **parameters** it contains. You can add the same **sample** to two **simulations** of different type (e.g. QE and SIESTA), and of course the resulting calculations (or **Job**s) will belong to different calculation engines.

DENEB's Project Browser: Quick reference guide

In **Project Browser** you control the actions by the use of its object's `context menus`. To **show the `context menu` of a given object**, first highlight it and then `Right-Click`.

Here is a **quick reference guide** to all different `context menus`, according to the object that they belong to:

- `Context menu` for **Root**:
  - Load all projects... : Loads a file that has been saved using Save all projects... .
  - Save all projects... : Saves the **whole Project Browser tree** in DENEB's efficient native format.
  - Create group... : Creates a new **group** under the **root**.
  - Create project... : Creates a new **project** under the **root**.
  - Paste group : Pastes under the **root** a copy of the **group** found in DENEB's **Clipboard**.
  - Paste project : Pastes under the **root** a copy of the **project** found in DENEB's **Clipboard**.

- `Context menu` for **Group**:
  - Create group... : Creates a new **group** under the highlighted **group**.
  - Edit group... : Edits the highlighted **group**'s label and description.
  - Delete group... : Deletes the highlighted **group**.
  - Create project... : Creates a new **project** under the highlighted **group**.
  - Create simulation... : Creates a new **simulation** under the highlighted **group**.
  - Create simulation from file... : Loads a valid input-file for some calculation engine, and creates a new **simulation** of the corresponding type. For example, from a SIESTA input file (with extension `.fdf`) , it creates a new SIESTA **simulation** under the highlighted **group**.
  - Copy group : Creates a copy of the highlighted **group** and places it into DENEB's **Clipboard**.
  - Paste group : Pastes a copy of the **group** found in DENEB's **Clipboard**.
  - Paste project : Pastes a copy of the **project** found in DENEB's **Clipboard**.
  - Paste simulation : Pastes a copy of the **simulation** found in DENEB's **Clipboard**.

- `Context menu` for **Project**:
  - Create simulation... : Creates a new **simulation** under the highlighted **project**.
  - Create simulation from file... : Loads a valid input-file for some calculation engine, and creates a new **simulation** of the corresponding type. For example, from a SIESTA input file (with extension `.fdf`) , it creates a new SIESTA **simulation** under the highlighted **project**.
  - Create group... : Creates a new **group** under the highlighted **project**.
  - Edit project description... : Edits the label and description of the highlighted **project**.

- Delete project: Deletes the highlighted **project**.
- Copy project: Places a copy of the highlighted **project** into DENEB's **Clipboard**.
- Paste group: Pastes a copy of the **group** found in DENEB's **Clipboard**.
- Paste simulation: Pastes a copy of the **simulation** found in DENEB's **Clipboard**.

- Context menu for **Simulation**:
  - Edit simulation...: Edits the label and description of the highlighted **simulation**.
  - Delete simulation: Deletes the highlighted **simulation**.
  - Copy simulation: Places a copy of the highlighted **simulation** into DENEB's **Clipboard**.
  - Import XMOL Sample...: Reads a file in XMol format (extension `.XYZ`) and creates a **sample** which is placed in the highlighted **simulation**. DENEB will detect if there is more than 1 frame in the file. In that case it lets you choose the type of loading: each frame considered as a new molecule, **or** each frame considered as a time step in the evolution of the same sample.
  - Copy sample: Places a copy of the **sample** in the highlighted **simulation** into DENEB's **Clipboard**.
  - `Paste sample`: Pastes a copy of the **sample** found in DENEB's **Clipboard** into the highlighted **simulation**.
  - Edit parameters...: Launches a new **Parameters Editor** that displays and allows to modify the **parameters** of the highlighted **simulation**.
  - Generate engine input file...: Creates a corresponding engine input-file using the data from the highlighted **simulation** (**sample** and **parameters**). The type of engine input-file obtained matches the type of **simulation**. For example, if the highlighted **simulation** is of the SIESTA type, DENEB will generate a ready-to-use `.fdf` file (SIESTA input file).
  - Run into engine...: Creates a **job** and launches it for execution into a given calculation engine. DENEB will show you a list with all the engine configurations currently defined for the given simulation type. After you choose one, DENEB will create and submit a new **job** to that specified machine (see **Job Manager**).

You will notice that the icon corresponding to the **simulation** just launched to "run into engine" changes.

Here is a list of possible icons for simulations that have been submitted and their meaning:

 = Submitted and waiting to be sent to the remote engine machine.

 = Simulation currently running in the remote machine.

 = Execution finished correctly (without any detected errors).

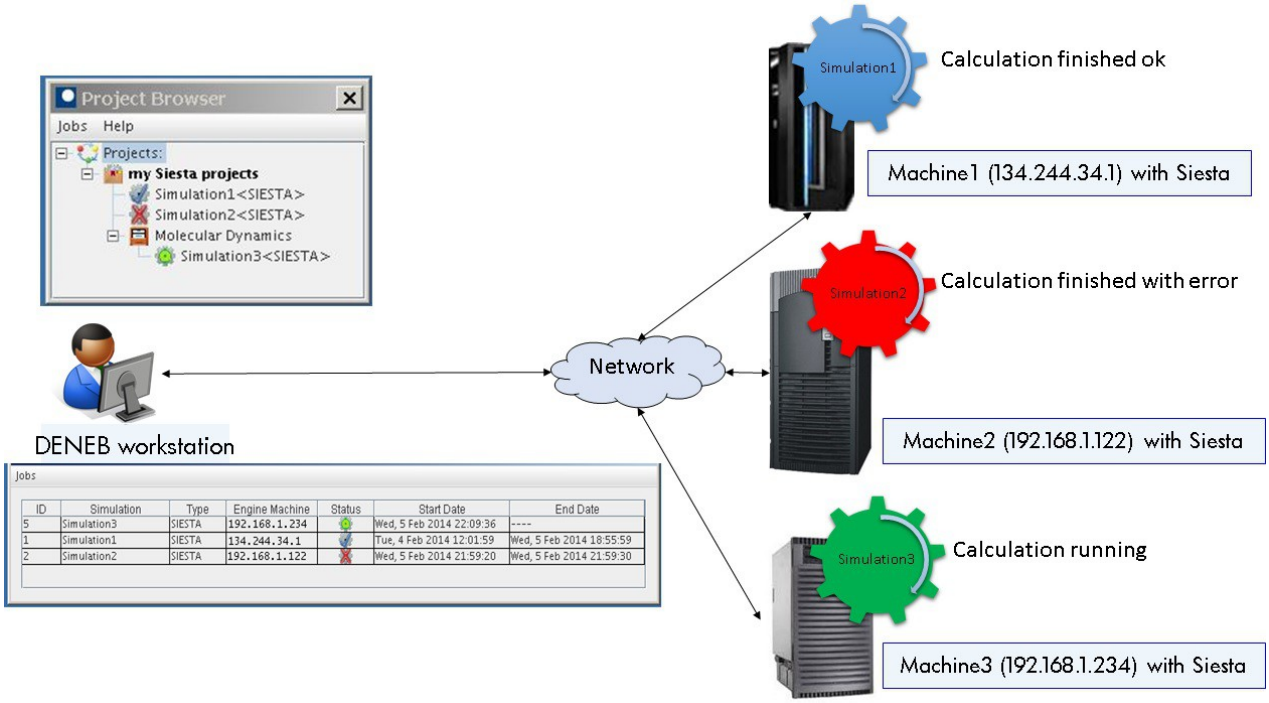
 = Execution finished with some detected error.

  - Kill simulation job: Halts and eliminates the associated **job** that is currently running in the remote machine (see **Job Manager**).
  - View engine output...: Retrieves and displays the current output file of the corresponding remote **job** (see **Job Manager**).
  - Preview-->Preview sample...: Shows a window in which the sample of selected simulation is displayed.
  - Preview-->Preview parameters...: Shows a window in which the computational parameters of selected simulation are displayed.

Drag and Drop:
In **Project Browser**, you can drag-and-drop objects to easily rearrange the tree. It is safe to experiment with drag and drop because when you attempt a non-valid motion (e.g., to move a **project** into another **project**) **Project Browser** will not complete such operation and will report about it.

DENEB's Project Browser: Defining engine configurations

DENEB's **Project Browser** can directly launch simulations for remote execution. But of course, DENEB needs to know some information about the *remote calculation engines* so it can connect and launch **jobs** on them. The following is an illustrative graph on how Deneb relates to different calculation engines in remote (or local) machines.



The set of data that defines a given executable in a given (remote) machine is called, in DENEB 's terms, an **engine configuration**. DENEB can store and use multiple **engine configuration**s. This is how you can define them:

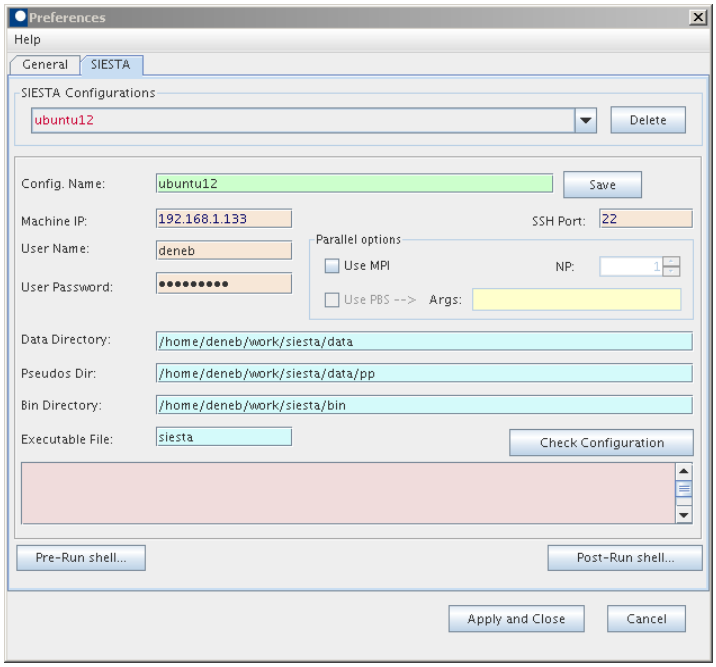
1. From DENEB's main window use Preferences → General and Plugins, you can also use the **main toolbar** short-cut button that looks like the following:

2. Fill out the requested information such as:
   a) IP : the IP address of the remote machine
   b) SSH port: port to use for the `ssh` connection.
   c) User name and User password: login information on the remote machine, the password field is not displayed and not susceptible to be copy-pasted.
   d) Parallel options: Select whether the executable is supposed to be launched for execution in parallel. Options are:
      1. Use MPI: check this box if you want the jobs to be submitted using `mpiexec` or `mpirun`.

2. NP: Input here the number of processors to be used.
3. Use PBS: check this box if the jobs are to be launched to a PBS type queue.
4. Args. : set here the particular arguments to be passed when launching to the PBS queue.

e) Executable File: Name of the executable file.
f) Bin Directory: absolute path where to find the executable file.
g) Data Directory: absolute path where to find write the data generated from simulations executions.
h) Pseudos Dir: absolute path where to find the pseudo-potential files.

For example, here is a possible engine configuration for SIESTA type simulations:



In the Siesta engine configuration you can freely define what bash shell commands will be run before and after the launching of the Siesta simulation. This way one can easily, for example, load MPI modules if needed. Use with care as any command would be run and there are potentially destructive uses of this features. Note the new buttons called Pre-Run shell... and Post-Run shell...

Checking an engine configuration:
The button Check Configuration triggers the verification of the data when pressed. Use it to verify the connection availability. If everything goes fine, an OK in a green background will appear, while a red background and an error message will be displayed if there is some connection trouble.

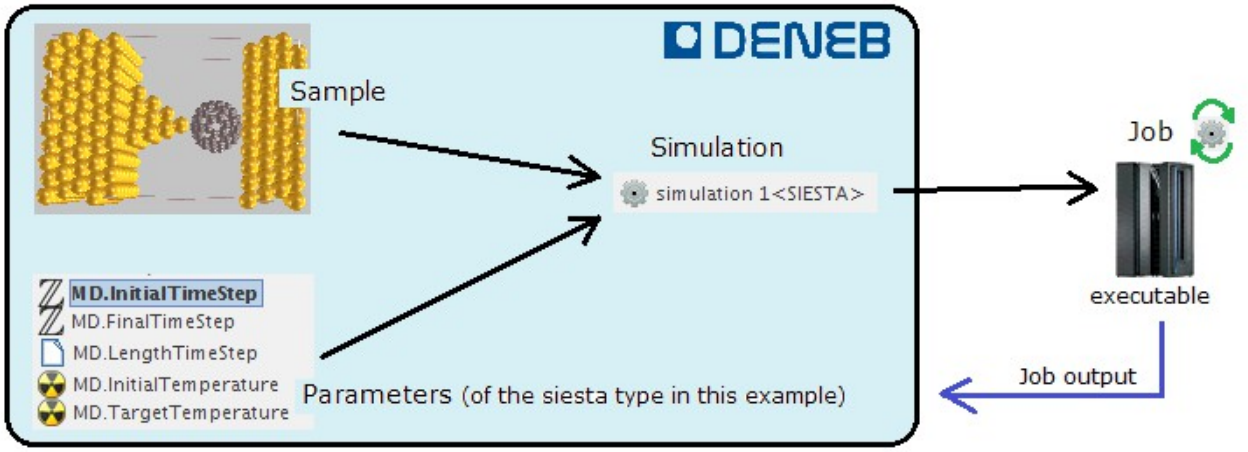
Note, make sure that your host can receive ssh connections: For example use "sudo apt-get install openssh-client" in an Ubuntu Linux, to install the ssh server.

The local computer can be also used as a calculation engine, provided that you install in it the proper calculation engine, **DENEB** will connect to it also using ssh and tcp/ip treated in the same way as remote hosts.

Project Browser's Job Manager

As we mentioned in previous sections, a **simulation** is composed of two parts: A **sample,** and a set *computational parameters*, the so-called **parameters**. The **parameters** is a set of pairs (label, value) that defines the needed input for a given particular **computational engine**. Note then that, while samples do not have particular association to any engine, simulations do since their parameters half belong to a particular engine. This way we talk of, for instance, SIESTA simulation, VASP simulation, etc ...

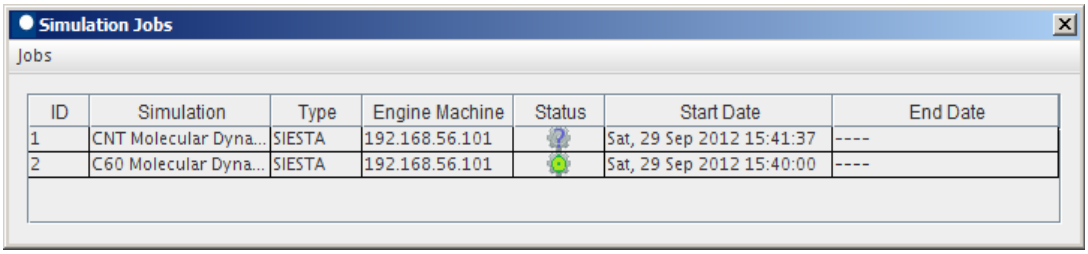
A simulation, becomes a **Job**, when it is launched to a (remote) machine for execution. DENEB automatically monitors all launched jobs, and lets you get the output-log (during and after the calculation with a single click. The **Project Browser's Job Manager** is in charge of facilitating all these tasks. It also facilitates the retrieval of all output files once the job has finished. The following diagram summarizes these processes:



Jobs can be in following status (represented in DENEB using different icons):

- Submitted and awaiting to be sent to the remote engine machine.
- Running in the remote machine.
- Finished correctly (without any detected error)
- Finished with some detected error

Job Manager allows you to quickly view the status of all your jobs by presenting them in a neat list, each row belongs to one job:



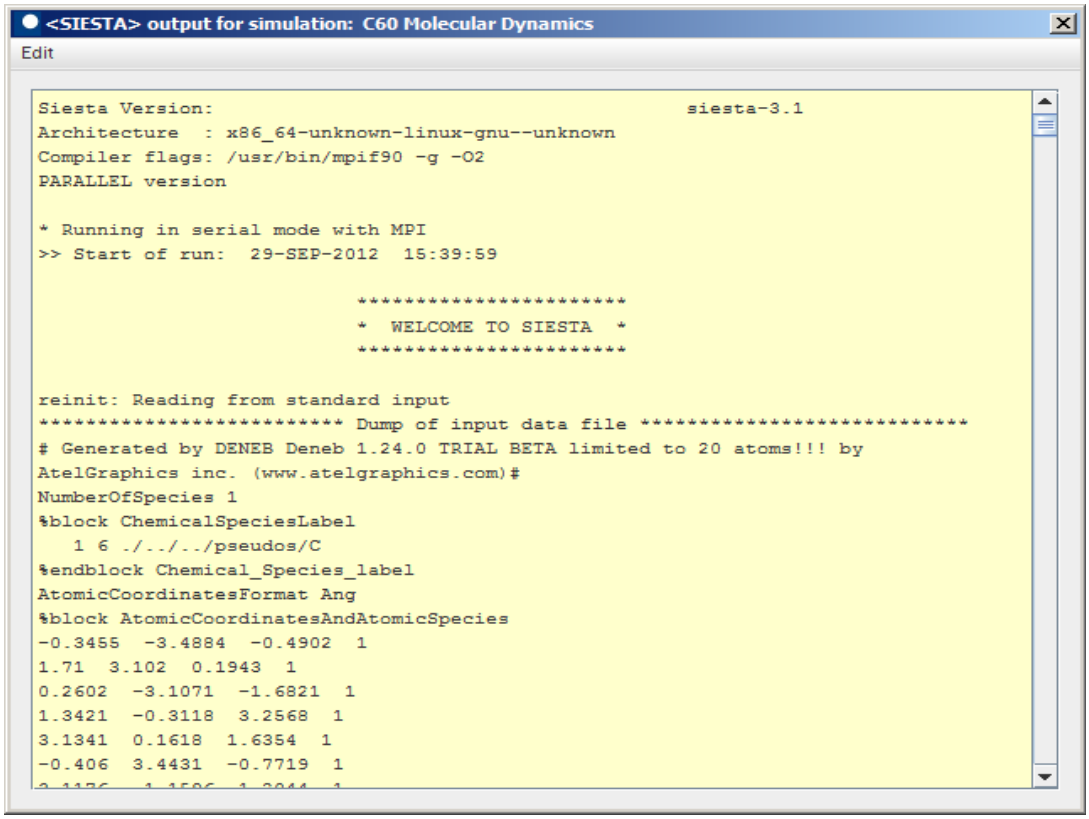
Job Manager shows in each row, the job's ID, the name of the associated simulation, the type of job, the TCP/IP address of the machine where it is being (or was) executed, its status (submitted, running, finished OK, finished with error), its starting time and date, and its ending time and date.

Using the menu called "Jobs" or the context menu of a given highlighted job, you can **kill the selected**

jobs, **view** the **content of the associated output-log,** and **retrieve the remote data files** to your local file system.

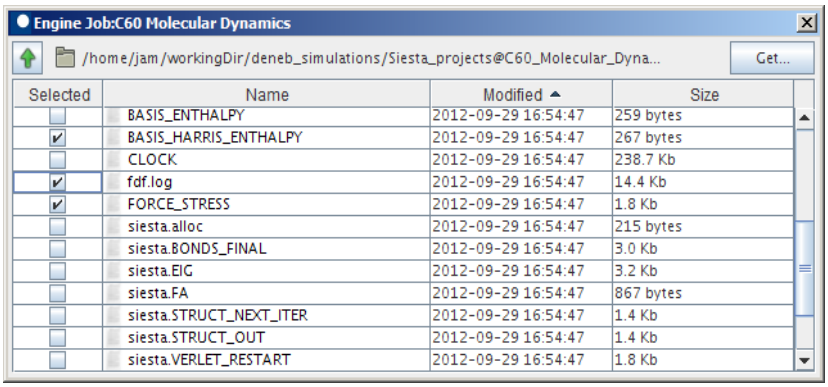
In the following we explain the actions for each of these menu items:

- Kill selected jobs: Tries to kill all highlighted jobs in their remote machines.
- View outputs...: Retrieves the output-logs from remote machine and shows them in a new window. Here is an example:



These windows show the status of the output log at the retrieval moment, to refresh the contents repeat the operation (trigger again the menu item called View outputs).

- Get remote data...: Shows the remote file system (files and directories) at the path where the associated job was executed. It lets you navigate in the remote file system (within the navigation permissions of the provided user):
  - Double-Click to enter a directory,
  - Press  to go up one level to the parent directory.
  - Use the check boxes at the left to select any number of items.
  - Press  to retrieve of the selected items from the remote file system to your local one.



DENEB's Parameters Editor

As we mentioned in previous sections, a **simulation** is composed of two parts: A **sample,** and a set *computational parameters*, the so-called **parameters**. The **parameters** is a set of pairs (label, value) that defines the needed input for a given particular **computational engine**. Note then that, while samples do not have particular association to any engine, simulations do since their parameters half belong to a particular engine. This way we talk of, for instance, SIESTA simulation, VASP simulation, etc …

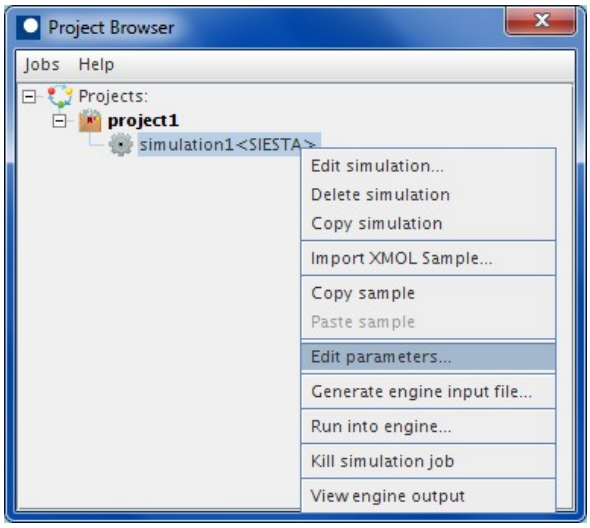
As we have seen, using **Project Browser** you can create a new simulation, provide it with a new sample (for example by pasting it from the **Clipboard**), and it will be directly ready to be click to launched for remote execution. This sends a default calculation for that sample and is sometimes all we need. The typical default calculation consist of computing the corresponding electronic density.

But for the most part we do require to change the default parameters so we can perform, for example, band structure calculations, mechanical relaxations, molecular dynamics, etc. To specify these **computational parameters** you can trigger the **Parameters Editor** from the context menu of any given simulation. When doing so, **DENEB** will start the editor corresponding to the type of simulation called for. Each plugin provides a new Parameters Editor so there are as many types of Parameter Editors as plugins you have in your system (not to confuse with "add-on"s. Remember each *plugin* enables the compatibility with a calculation engine, while *add-ons* are features that you can add to **DENEB** not specifically linked a calculation engine).

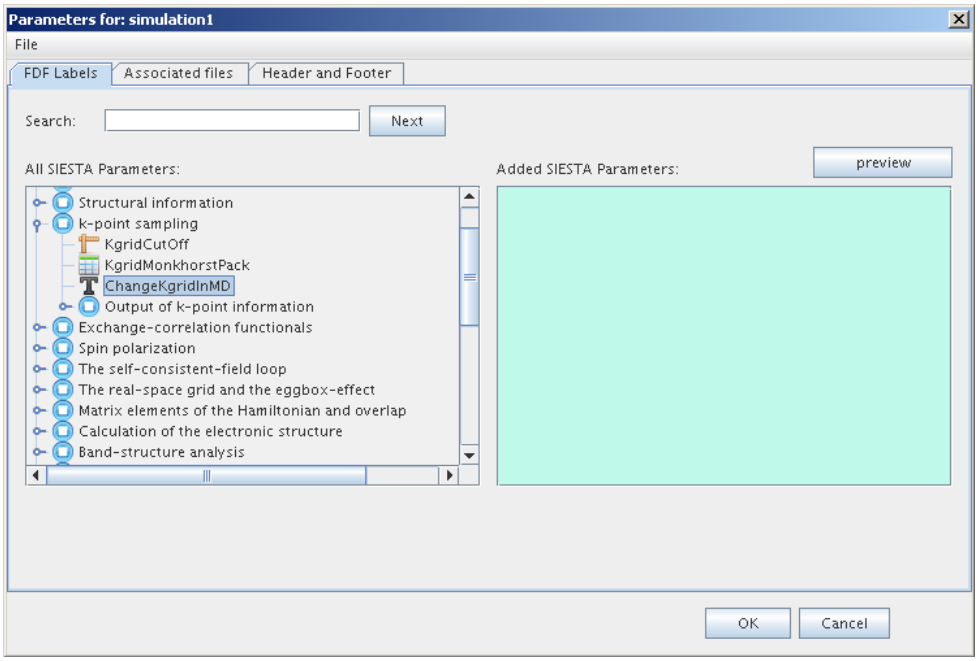
In the following we describe the workings of the different **Parameter Editors**:

DENEB's SIESTA-Parameters Editor

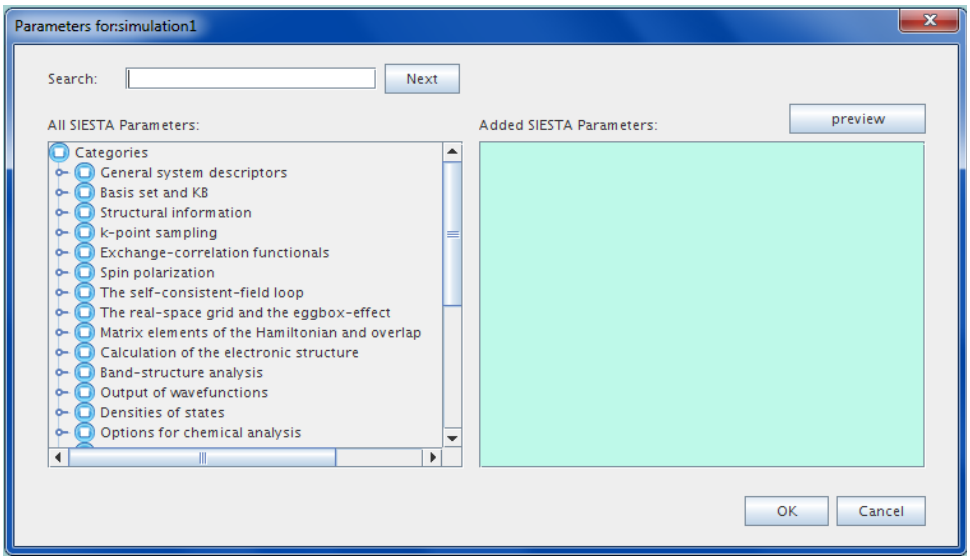
To trigger its appearance use the context menu of a simulation of the type SIESTA, within the **Project Browser** tree. Choose Edit parameters…



This will produce the siesta-Parameters Editor. That looks like this for a newly created simulation:

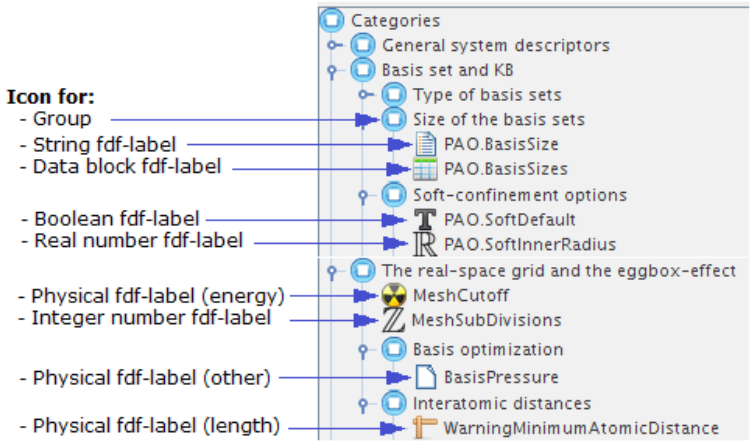


It has three associated tabs, as you can see. The first one called fdf-labels contains the following:



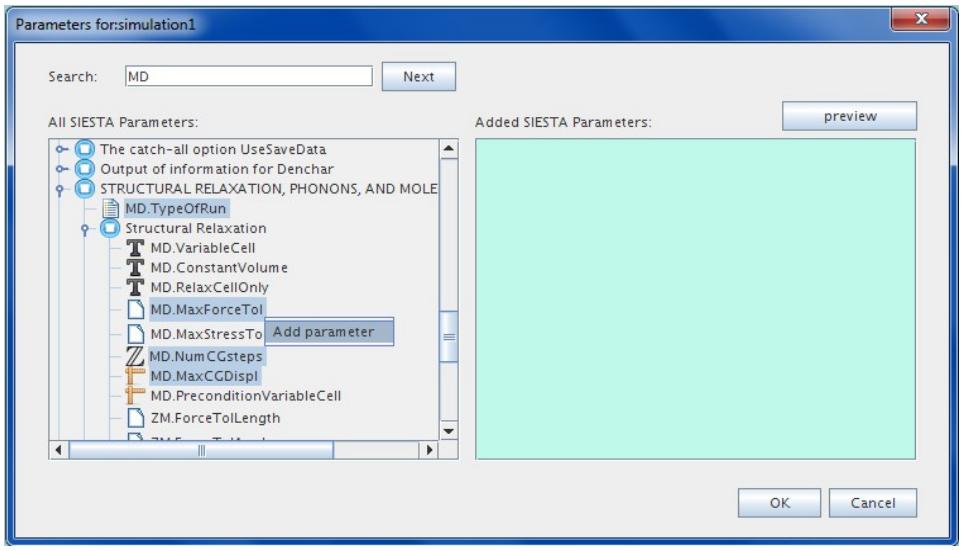
It mainly consists of two panels, on the left you can find in a tree-organization all the available siesta-fdf labels (Deneb 1.26 comes with all labels for its contemporary siesta 3.1). The tree organization reflects the organization of the siesta users manual, this way you can quickly find the documentation of any given label in the same. For quick-search of fdf-labels you can type any (case sensitive) text in the corresponding box (labeled `Search`) and press the button labeled `Next`; this will find and highlight the first appearance, as you repeatedly press `Next` the following appearances of the text will be highlighted.

The icons in the tree give you quick visual clues as to what kind of item each branch/leaf corresponds. In the following figure we specify the item type for all different icons:

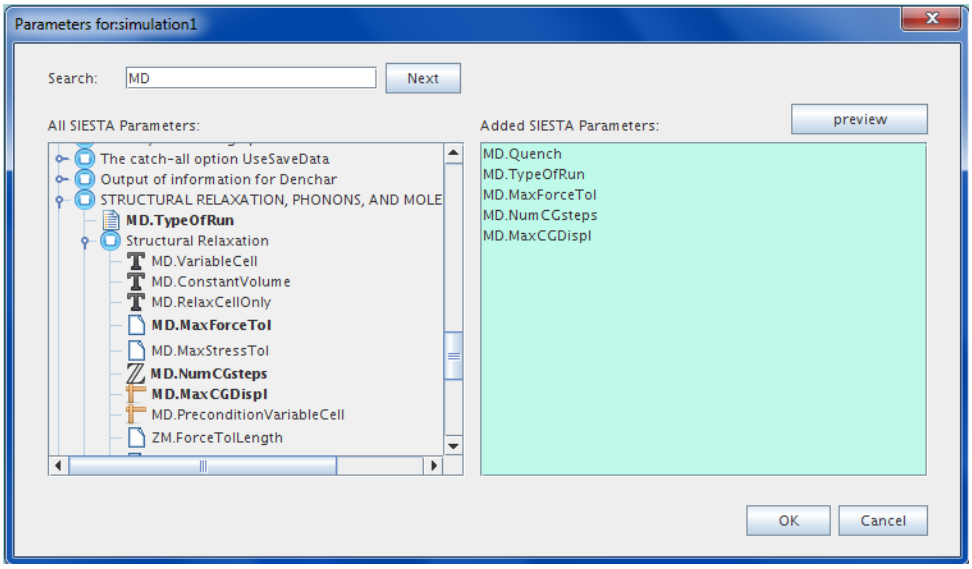


Note: The fdf-labels that specify the sample (such as: number of atoms, atomic coordinates, chemical species, lattice vectors etc) are not present in the **Parameters Editor** tree. Obviously this is because they are not necessary here since they are already determined by the sample included in the corresponding simulation.

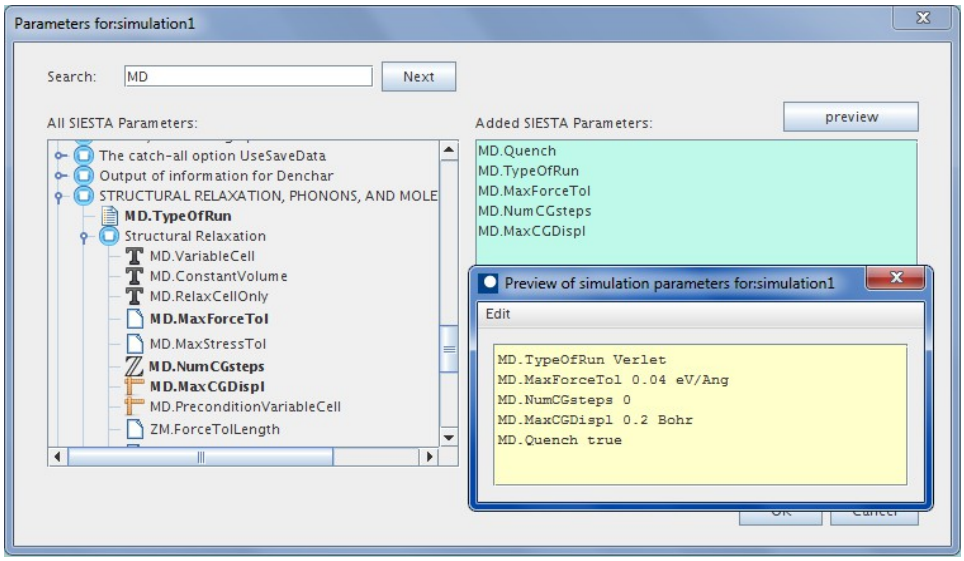
When submitting a simulation for execution, **DENEB** creates a corresponding **engine input-file** (a siesta fdf file in this case). This engine input-file includes both labels that define the sample and labels that determine the computational parameters. The siesta engine can take default values for all computational parameters but those of the sample, so a perfectly valid set of computational parameters is an empty one. Nevertheless in most occasions one needs to specify some different (from the default) values. The way to do so is to "Add" the corresponding parameters to the right hand side panel. Use the context menu of the highlighted set of computational parameters to add them:



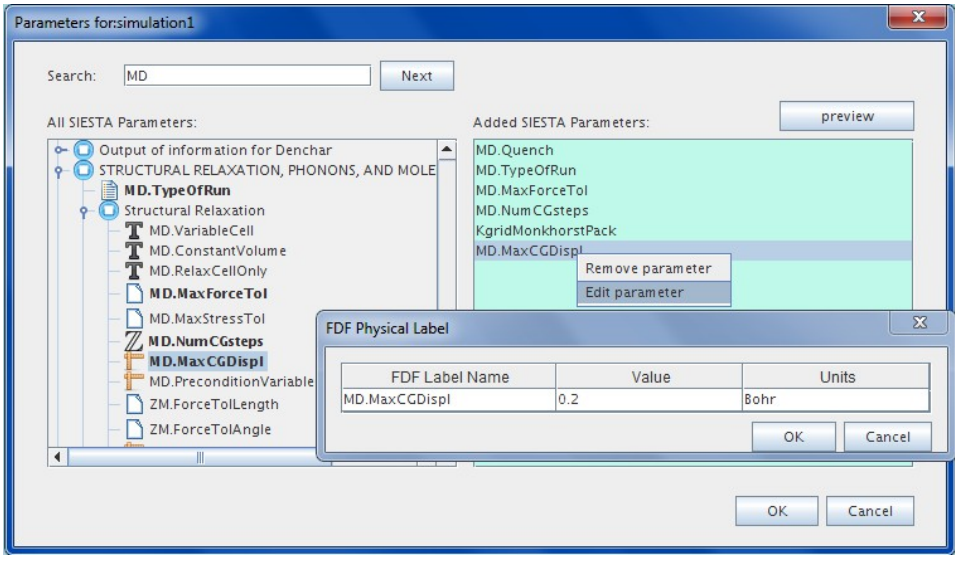
You can add one or several with one click, if you highlight a branch all of the parameters under such branch will be added. Obviously you can add all parameters by using the context menu of the tree root branch (labeled "`Categories`"). The added labels appear in the right hand side panel and are written with bold face characters in the tree.



In order to view the current status of our added set of parameters we can use the button labeled preview. By pressing it an overview of all the added labels and their current values is shown.

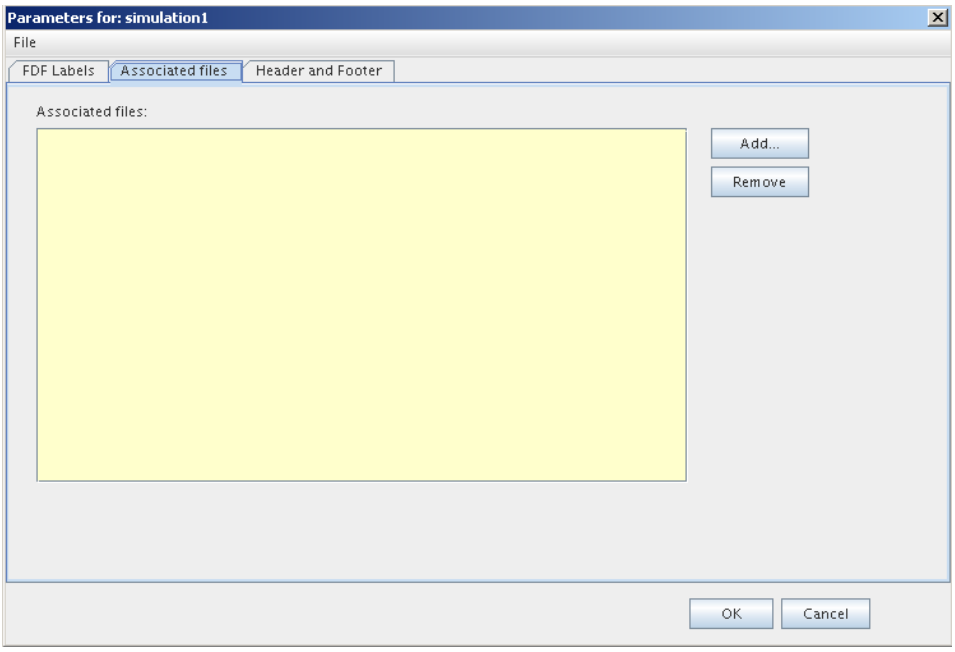


You can view and modify specific labels from those that have been added by using its context menu (triggered by Right-Click). You can type in new values and or units it and press OK to make it count or cancel to disregard it. Note: once you press OK there is no undo, so use with care. If you input not a number, where a number is expected, **DENEB** detects so and does not register the OK press. If you input units not recognized by siesta, they will be disregarded upon pressing OK, and the units field will not be changed. Note however, that the parameters checking provided by **DENEB** is not foolproof and it does not check for unreasonable sets of parameters from the Physics viewpoint.



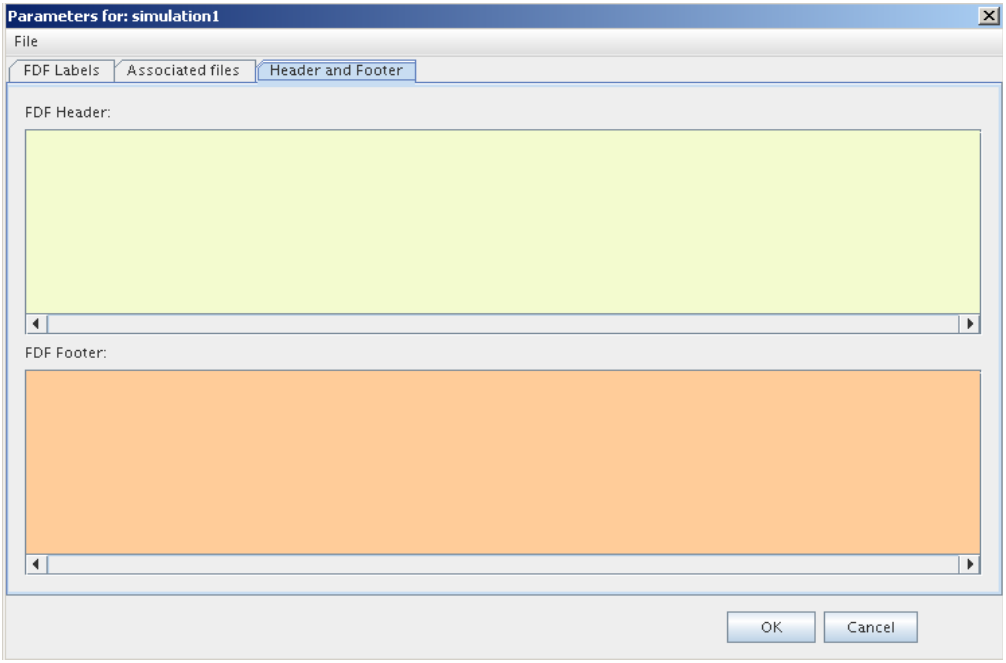
Finally, when you are done viewing/editing the parameters press the button OK in the parameters editor window to actually register the changes and modify thereby the corresponding simulation's parameters. If you regret of all the changes done you can still press "Cancel" and the simulation parameters will remain unchanged. The **Parameters Editor** window disappears upon pressing OK or Cancel, you can obtain a new one again by the simulations context menu item Edit parameters... as explained above.

The next tab is called Associated files and it looks like this:



Here you can add one or several files that will be copied (using ssh protocol) to the directory where the executable of siesta is placed. Then, siesta will be called for execution (either directly in bvackground, or using mpi, or using PBS, as a function of the particular engine configuration used). The goal of this tab is that if you need for siesta to use some specific files at running time, you can deliver them here to the remote host.

The final tab looks like this:



In it you can freely write any text that will be added to the header (top) and footer (bottom) of the fdf

file that will be sent to the remote host. Its use is for example to add extended comments, or for example add those fdf labels that are particular of your siesta modified engine and therefore can not be found in the standard list of fdf files (first tab of Parameters Editor).

Finally note that in the **siesta Parameters Editor** a new menu called File has been added. You can now easily save and recover your favorite set of default values for all fdf labels, use for that purpose the new menu items called File → Load template , and File → Save as template. The latter will store in a file your whole set of current fdf labels (added or not) and the former will recover them. This way you can quickly load you set of default values for your fdf labels as you have them stored in a file.

DENEB's video-demos

DENEB's YouTube videos

One picture is worth a thousand words. And a video is about 24 pictures per second. In Atelgraphics YouTube channel you can find some video demonstrations and tutorials about **DENEB**. Sometimes the faster way to learn is to see it done, check the `atelgraphicschannel` regularly.

Here you have a relatively short list of links, the number of these will steadily grow.

1. A short video of the visualization of the results of a molecular dynamics (MD) simulation with **DENEB**, water over a Pt surface. Water dissociation over Pt. One minute.
2. A complete demo. Learn it all in only 13 minutes: Create a sample, modify it, include it in a simulation, execute it remotely, retrieve the results and visualize the MD animation. Gold dimer into C60 complete.
3. Another demo on how to visualize an animation resulting from a MD simulation. Iron atoms inside a Carbon nanotube. Six minutes.
4. Today Quantum Dots (QDs) have been projected as one of the most relevant nanostructures for the implementation of high efficiency photovoltaic and optoelectronics devices. With **DENEB** you can easily build any kind of quantum dot. This video shows an example: in only 5 minutes, starting from scratch, a Gallium Arsenide Quantum Dot is built, classified, and stored for later use in DFT simulations.
5. A step by step complete setup process. In only 12 minutes learn to install and tune all the necessary to convert your windows PC in an independent graphical ab-initio Molecular Dynamics machine, where the intelligent front end is **DENEB** and the powerful calculation engine is Siesta (DFT calculation software). Ideal if you want to carry in your laptop a complete software for (small) ab-initio simulations that you can graphically prepare, launch and visualize. The video shows you how to install the virtual machine software, a Linux system on it, the siesta engine on it, and how to install **DENEB**.
6. Gold Nanoparticles have emerged as a promising scaffold for Targeted Drug Delivery due to their affinity to organic molecules and their low toxicity. This is important, for example, for new treatment approaches to some types of cancer. This video shows a Quantum Molecular Dynamics simulation prepared using **DENEB** (and siesta as the calculation engine). Note how the ibuprofen molecules stick to the gold cluster remaining nevertheless integral and chemically active.
7. A supersonic gold "bullet" hitting a C60 caging a gold atom. This molecular dynamics simulation performed with **DENEB** - Siesta, shows how in the nano-world 2000 Km/h (quicker than the typical speed of a bullet) does not look so fast. The gold-atom supersonic bullet bounces back on the C60-Au target.

DENEB's older video-tutorials

(**Note**: the following video tutorials are for version 1.2 of **DENEB**,
but still useful to learn many concepts.)

NanoExplorer

To see a demonstration of **NanoExplorer**'s basic use, there is a tutorial in the "`Downloads`" section of the Atelgraphics web site. It is entitled "*NanoExplorer Essentials*"

In that tutorial you may learn the following:

- How to **invoke NanoExplorer**
- How to **rename**, **delete**, **visualize** and **copy** samples in **NanoExplorer**.
- How to **count the number of molecules and atoms** in a given sample.
- How to **save the looks of a sample** in an *jpg* file.
- How to **copy** a given sample from **NanoExplorer** into DENEB's **Clipboard**.
- How to **quick search** for samples by (parts of) their name.
- How to **tell periodic from molecular sample types**.
- How to **import and export** samples in different formats.
- How to **quickly arrange several simultaneous views** of several samples.
- How to quickly **create a new simulation** using a sample from **NanoExplorer**.

Project Browser

To see a demonstration of **Project Browser**'s basic use there is a tutorial in the "Downloads" section of the Atelgraphics web site. It is entitled "*Project Browser Essentials*"

In that tutorial you may learn the following:

- How to **invoke or show Project Browser.**
- How to **create a new project, set its description and (re)name it.**
- How to **create groups and move projects into them.**
- How to **load or save all groups and projects at once.**
- How to **edit projects and groups**.
- How to **create simulations under projects.**
- How to **copy/paste, eliminate groups, projects, simulations.**
- How to **edit, delete, copy simulations.**
- How to **import an *XYZ* file into a given simulation.**
- How to **directly edit the sample of a simulation.**
- How to **directly edit the computational parameters of a simulation.**
- How to **generate an "engine input file" ready to be fed to a calculation engine.**
- How to **send a simulation for remote execution into a given engine.**
- How to **kill a remote running job belonging to a particular simulation**.
- How to **visualize the output after a given simulation has successfully run.**

Sample Manipulator: invoking

To see a demonstration of **Sample Manipulator**'s several simultaneous instances management, there is a tutorial in the "Downloads" area of the Atelgraphics web site. It is entitled "*Invoking Sample Manipulator*"

In that tutorial you may learn the following:

- How to **invoke or show several instances of Sample Manipulator.**
- How to **eliminate some of the instances created.**
- How to **view the list of the currently active Sample Manipulator instances.**
- What is the meaning of **the order in which the different instances may appear in the list**.

Sample Manipulator: Mouse Drag Mode

To see a demonstration of **Sample Manipulator**'s camera control in the *Mouse Drag mode* there is a tutorial in the "Downloads" area of the Atelgraphics web site. It is entitled "*Mouse Drag Mode in Sample Manipulator*"

In that tutorial you may learn the following:

- How to **quickly show all windows of Sample Manipulator.**
- How to **resize 'main view' and 'side view' using the split panel.**
- How to **zoom in/out of the detached view panel.**
- How to **add a new sample chosen from the Sample Manipulator's Palette.**
- How to **set the *Mouse Drag* mode for camera control.**
- How to **control rotation, zoom and shift of the camera in the Mouse Drag mode.**
- How to **change the 'center of camera rotation' by mouse picking a point in space.**
- How to **control the position of the auxiliary plane in this (and all) mode.**

Sample Manipulator: Sliders and buttons mode

To see a demonstration of **Sample Manipulator**'s camera control in the *Sliders and Buttons mode* there is a tutorial in the "Downloads" area of the Atelgraphics web site. It is entitled "*Sliders and Buttons Mode in Sample Manipulator*"

In that tutorial you may learn the following:

- How to **set the Sliders and buttons mode.**
- How to **zoom in and out** in this mode.
- How to **reset the view** to a default position.
- How **shift step by step** the camera.
- How to **create new samples picking them from the Palette**.
- How to **display the coordinate axes**.
- How to **rotate the camera using the progress bars, spinners, and typing angle values**.
- How to **rotate around each different axis**.
- How to **shift the camera position by mouse-drag**.
- A tip to better compare samples: How to **accurately specify the same view point**.
- How to **control the side view panel camera**.
- How to **dock/undock, and resize the detached view panel**.
- How to **control the detached-view camera: shifts and zooms**.
- How to **reset to default the view of the detached-view panel**.
- How to **dock all Sample Manipulator's side windows**.
- How to **exit a Sample Manipulator instance destroying its memory content**.

Sample Manipulator: Simple building

To see a demonstration of **Sample Manipulator**'s abilities to build from scratch there is a tutorial in the "Downloads" area of the Atelgraphics web site. It is entitled *"Sample Manipulator: Building simple samples"*

In that tutorial you may learn the following:

- A short-cut **to show all Sample Manipulator's windows**.
- How to **choose a sample from the Palette**.
- The **use of the Empty Sample** of the Palette.
- How **the Sample Manager offers a tree view** of the samples.
- How **to rename the samples and molecules** using the Sample Manager.
- How to **set a molecule/sample as 'the one being edited'**.
- How to **choose an specific atom from the Palette**.
- How to **add atoms by mouse actions using the plane**.
- How to **select all atoms using the Selection menu**.
- How to **edit the current selection**.
- How to **type new coordinates for a given atom in the Atom Editor**.
- How to **add a just built sample to the Palette** (that has persistence functions).
- How to **place clone copies of a given sample by mouse actions**.
- How to **quickly visualize coordinates in the Sample Manager tooltips**.

Sample Manipulator: Building periodic samples

To see a demonstration of **Sample Manipulator**'s abilities to build from scratch periodic samples there is a tutorial in the "Downloads" area of the Atelgraphics web site. It is entitled *"Sample Manipulator: Building simple periodic samples"*

In that tutorial you may learn the following:

- How to **use the Empty sample from the Palette**.
- How to **place a sample at an specific point**.
- How to **make a sample periodic**.
- How to **find an atom in the Palette**.
- How to **place an atom by mouse picking**.
- How to **rename a sample/molecule**.
- How to **set a sample/molecule as the one being edited**.
- How to **display the coordinate axes**.
- How to **select an atom by mouse ctrl-clicking**.
- How to **edit the atom's scaled coordinates by using the Atom Editor.**
- How to **tag an atom with a customary label**.
- How to **obtain information from an atom viewing the Atom Editor tool tips**.
- How to **edit a sample's unit cell parameters** (to set them as an FCC lattice, in this case).
- How to **add to the Palette a just created sample**.
- How to **create a supercell sample from a given sample**, by repetitions along the lattice vectors.
- How to **choose a new center of camera rotation by mouse picking**.

Running simulations

To see a demonstration on **how to launch for execution a just created simulation** there is a tutorial in the "Downloads" area of the Atelgraphics web site. It is entitled "*Running simulations*"

In that tutorial you may learn the following:

- How to **set the parameters relative to the remote host** where the simulations will be run.
- **What parameters are needed** in order to instruct DENEB about said remote host.
- How to **create a new project in Project Browser**.
- How to **create a new simulation under a project**.
- How to **bring a sample from the NanoExplorer database into the just created simulation**.
- How to **short-cut visualize, as a tooltip, the sample contained in a simulation**.
- How to **edit the computational parameters of the simulation**.
- How to **select specific parameters and edit them using Parameter Editor**.
- How to **preview the parameters section** (not containing the sample) **of the engine input file**.
- How to **generate an engine input-file** that can be directly sent to the calculation engine.
- How to **instruct DENEB to: generate the input file, deliver it to the remote host, and start the simulation in the remote host.** With a single click.
- How to **view a summary of the jobs that have been launched** for execution using the **Job Manager.**
- **What icons uses DENEB to indicate different statuses of the launched simulations**.
- How **the main panel status bar shows information about the latest submitted job**.
- How **DENEB detects when the remote job has finished and, if successful, retrieves the output**.
- How **the status of a job is shown both in the Project Browser and in the Job Manager**.
- How **to view the output file of a finished simulation**.

DENEB's cheat-sheets

Sample Manipulator: Mouse actions cheat-sheet

	Pick Mode: **Atoms**.	Pick Mode: **Molecules**.	Pick Mode: **Samples**.
Left-Click	A new atom, whose type is the one highlighted in the **Palette**, is created. Its center (nucleus) is placed on the spot of the plane touched by the mouse cursor. The newly created atom belongs to the *molecule being edited,* that should have been set using the **Samples Manager**. (Only **if** Plane: **Visible.** Otherwise, nothing done)	A new molecule, of the type highlighted in the **Palette**, is created. Its reference point (the point with respect to what its atom's local-coordinates are defined) is placed on the spot of the plane touched by the mouse cursor. The newly created molecule belongs to the *sample being edited,* that has been set using the **Samples Manager.** (Only **if** Plane: **Visible.** Otherwise, nothing done)	A new sample, of the type highlighted in the **Palette**, is created. Its reference point (the point with respect to what its molecule's local-coordinates are defined) is placed on the spot of the plane touched by the mouse cursor. (Only **if** Plane: **Visible.** Otherwise, nothing done)
Ctrl + Left-Click	If the mouse cursor is touching a given atom. Its selection state is toggled. Otherwise, nothing done.	If the mouse cursor is touching a given atom. The selection state of **all atoms in its molecule** are toggled. Otherwise, nothing done.	If the mouse cursor is touching a given atom. The selection state of **all atoms in its sample** are toggled. Otherwise, nothing done.
Shift + Left-Click	If the mouse cursor is touching a given atom. It is eliminated. **Note: there is no warning or undo.** Otherwise, nothing done.	If the mouse cursor is touching a given atom. Its whole **molecule** is eliminated. **Note: there is no warning or undo.** Otherwise, nothing done.	If the mouse cursor is touching a given atom. Its whole **sample** is eliminated. **Note: there is no warning or undo.** Otherwise, nothing done.
Shift + Right-Click	Place the camera rotation center at the point of the plane touched by the mouse cursor. (Only **if** Plane: **Visible.** Otherwise, nothing done.)		
Left-Click & Drag	Camera rotation depending on the drag direction. (**If** Preferences → Camera Control Setting = Mouse Drag**.**)		
Right-Click & Drag	Camera shifts laterally with the mouse motion. (**If** Preferences → Camera Control Setting = "Mouse Drag" **or** "Sliders and buttons".)		
Center-Click & Drag	Camera zoom in and out depending on the **vertical** drag direction. (**If** Preferences → Camera Control Setting = Mouse Drag**.**)		
Ctrl + Shift & Move Cursor	Tooltip with the coordinates of the point **at the plane** touched by the mouse cursor. (**If** Preferences → Graphical tooltip options = See coords on the plane) Tooltip with the coordinates of the **point at the plane** touched by the mouse cursor **or** information about the **atom** touched by the mouse cursor. (**If** Preferences → Graphical tooltip options = Coords on plane and atoms info)		
Mouse-Wheel Rotation	Camera zoom in/out step by step. (**If** Preferences → Camera Control Setting = "Mouse Drag" **or** "Sliders and buttons".)		

Sample Manipulator: Key navigation camera controls.

This is a reminder of the keys that control the motion of the camera in the Key-Navigation mode: Preferences → Camera control setting → Navigation Keys.
This mode is particularly useful when:

- You want to navigate inside hollow samples.
- You want to quickly 'overfly', surfaces or elongated samples.
- You want to zoom-in beyond the center of rotation.
- You prefer to quicker zoom in or out with pressing keys rather than using mouse wheel repeated actions.
- In general, when you need camera traveling in long (but still nanometric!) distances.

	Action performed when camera control mode = **Navigation Keys** (Preferences → Camera Control Setting = **"Navigation Keys"**)
Q	The camera moves forward.
A	The camera moves backwards.
Up - Arrow	The camera rotates upward.
Down - Arrow	The camera rotates downward.
Right - Arrow	The camera rotates to the right.
Left - Arrow	The camera rotates to the left.
Ctrl + Up - Arrow	The camera shifts upward.
Ctrl + Down - Arrow	The camera shifts downward.
Ctrl + Right - Arrow	The camera shifts to the right.
Ctrl + Left - Arrow	The camera shifts to the left.

DENEB-1.28. Known issues

1. **"Out of memory" issue:** The 32 bits version can address 2Gb of RAM maximum. This means that when the user has opened (visualized) samples that together add up to about 20K atoms DENEB might exit unexpectedly with an out of memory uncaught exception. Beware therefore when visualizing bulky or numerous samples with NE or SM, save your work frequently just in case. This does not happen with the 64 bits versions.