Table of Contents

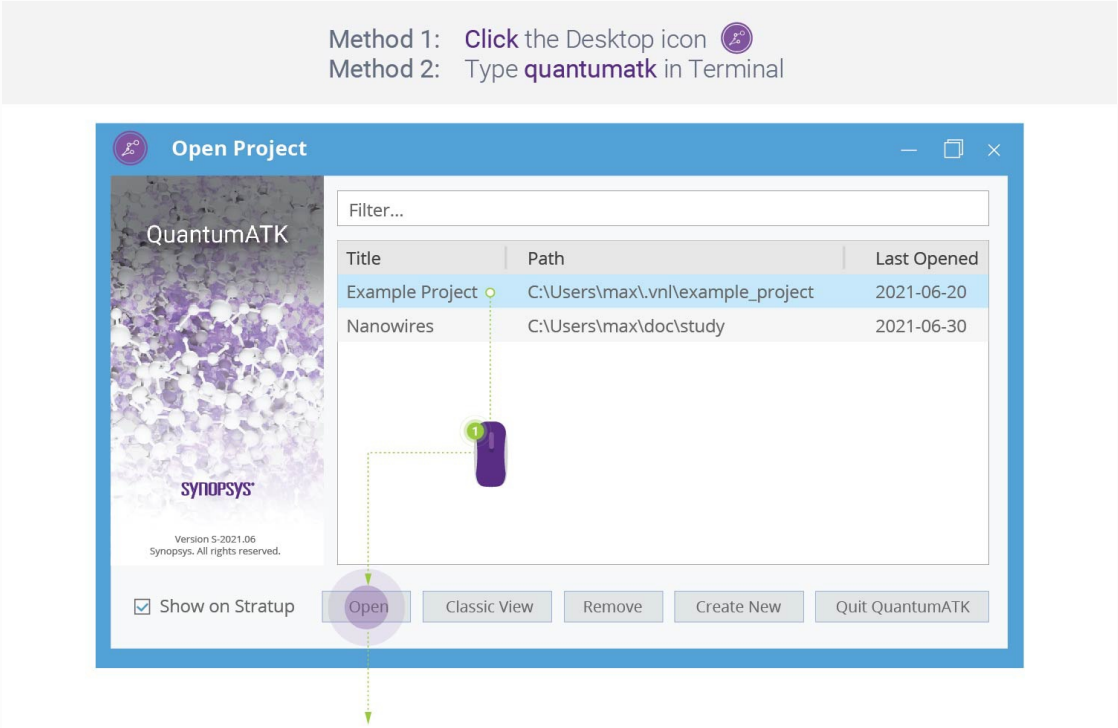
Table of Contents 1
Getting Familiar with QuantumATK 2
- QuantumATK Main Window 2
  - Menu Bar 3
  - Vertical ToolBar 3
- Building Atomistic Structures 4
- Script Generator 6
- Job Manager 7
- Analyzing the Results 8

Getting Familiar with QuantumATK

There are two different ways to start up QuantumATK:

1. by clicking the QuantumATK icon on the Desktop;
2. by executing the `quantumatk` command in a terminal.

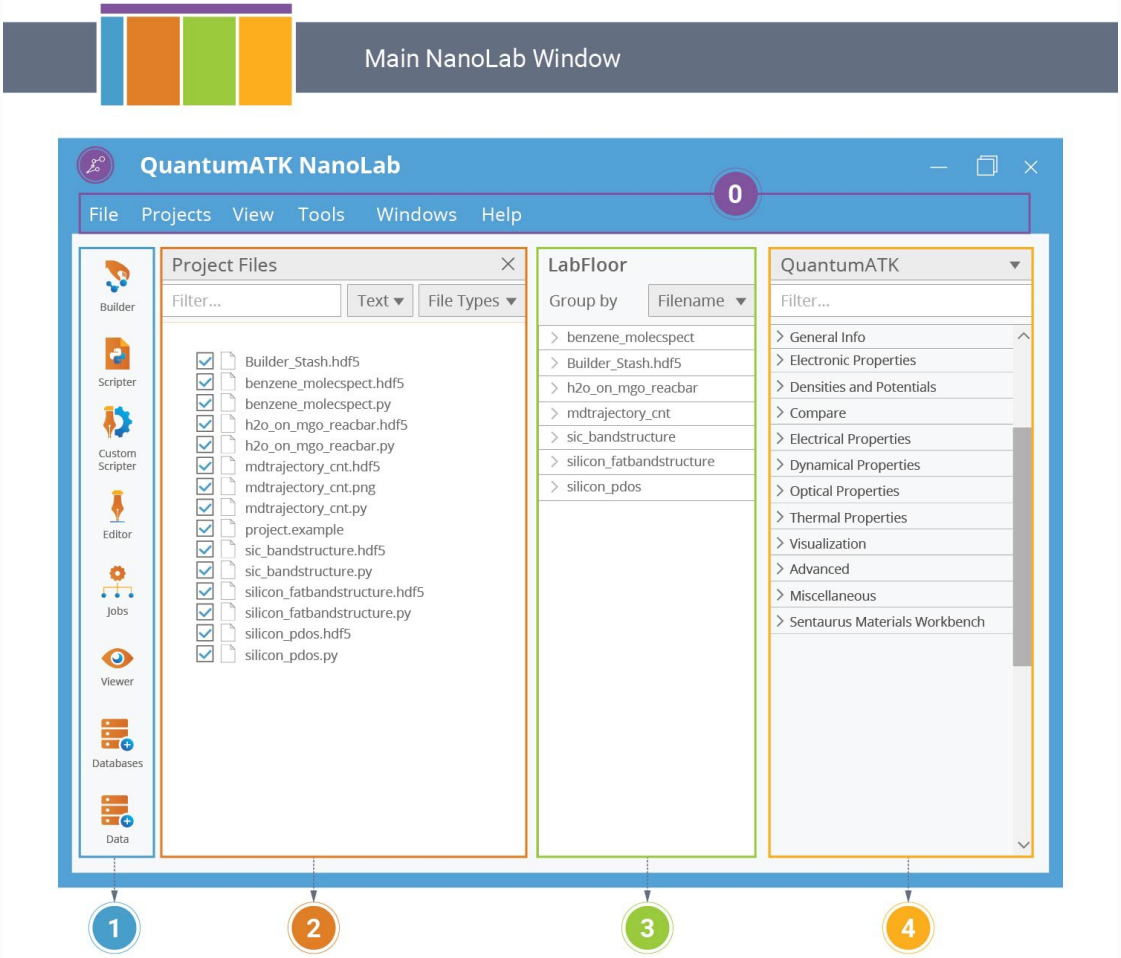
When doing one of these, the **Open Project** window will appear. It allows you to manage projects and open one of them. Each project must be given a suitable title and a local path for storing project files. Use the **Create New** button to add a new project (see next chapter).



Once you have selected a project and clicked **Open**, the QuantumATK main window will show up. The following sections will introduce the main parts of QuantumATK and the functionalities each part offers.

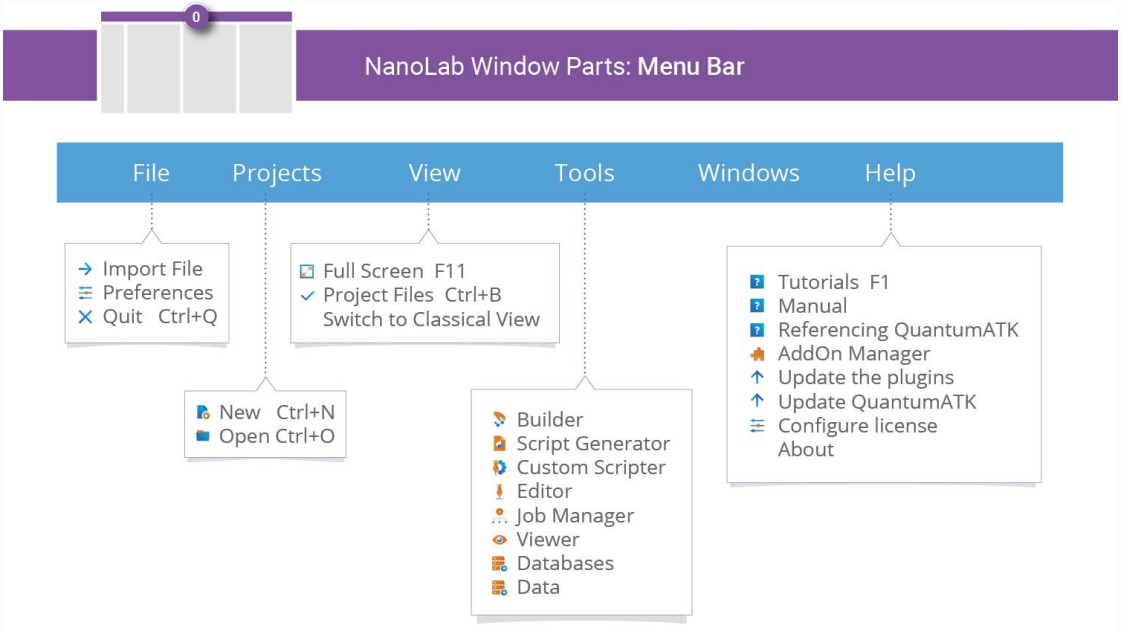
QuantumATK Main Window

The figures below illustrate how the QuantumATK main window may be divided into 5 main sections.



Menu Bar

The Menu Bar is the horizontal bar located at the top of the main window. Use it for example to import files, open new projects and quit the program. The bar also allows you to open the Preferences, About QuantumATK, and AddOns Manager widgets.



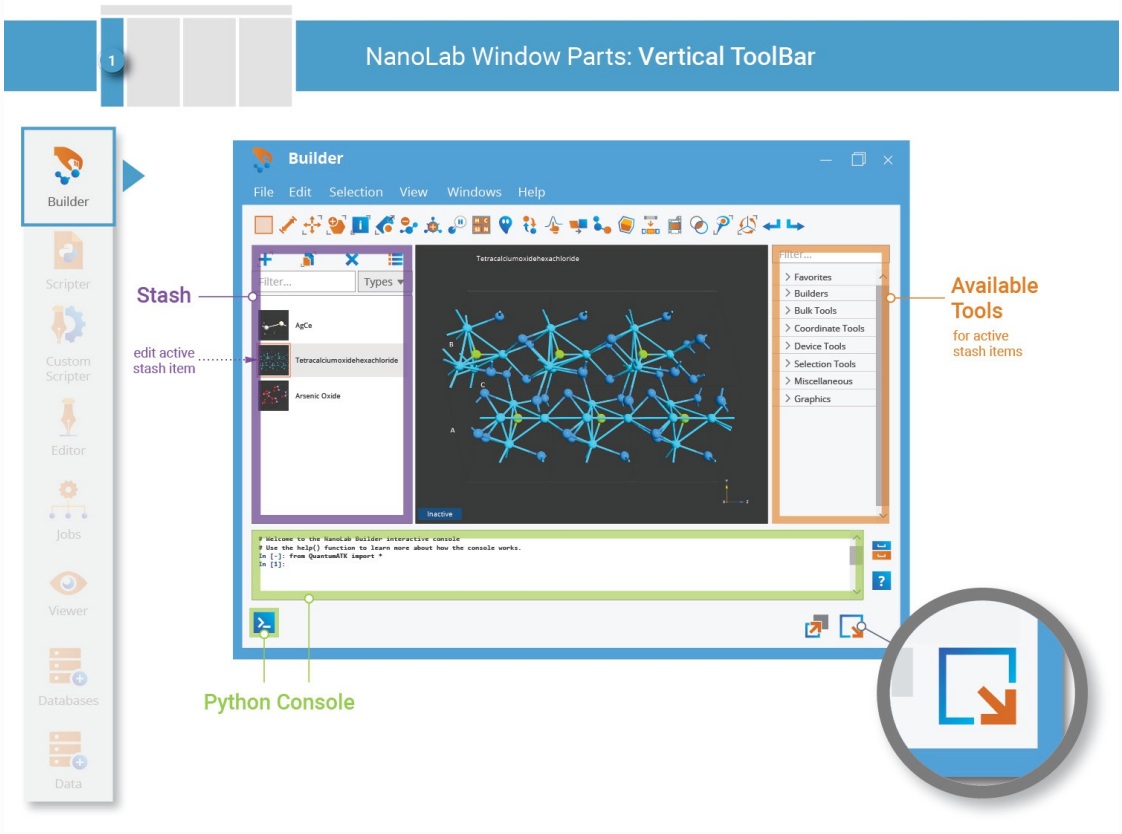
Vertical ToolBar

The combination of QuantumATK, and Python scripting is extremely flexible, and makes it possible to do your everyday atomistic modeling in a variety of different ways. However, the design of QuantumATK encourages in particular one simple and intuitive **workflow**:

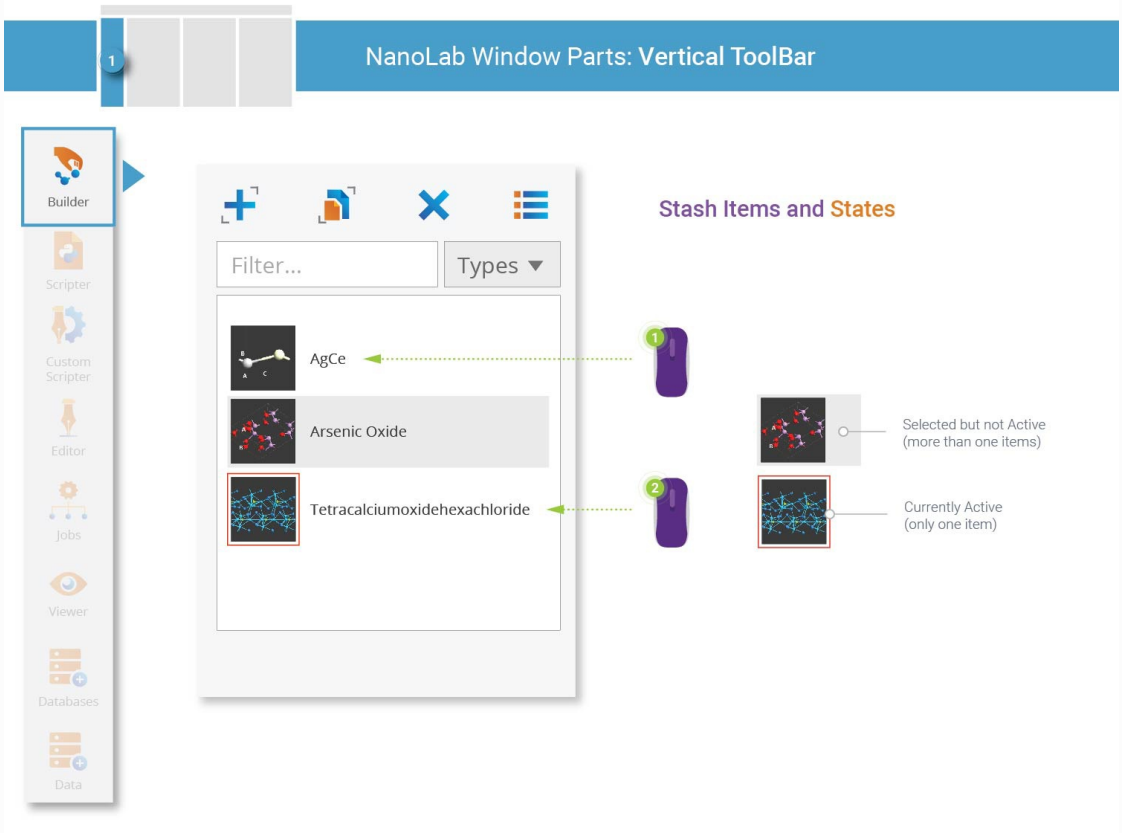
1. Create atomistic structure.
2. Set up calculations.
3. Run job.
4. Analyze results.

Building Atomistic Structures

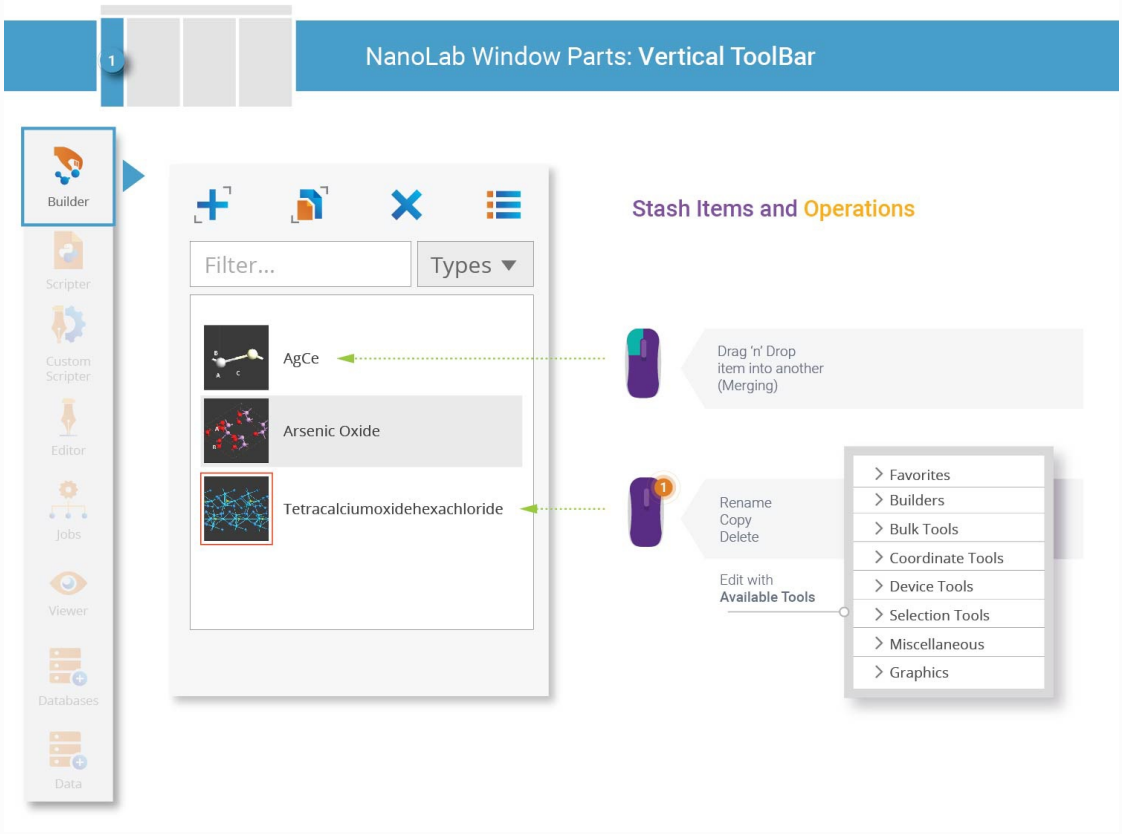
The **Builder** is a graphical interface for building any desired nanoscale structure. The **Stash** contains the configurations you have built in the current project, and an ever expanding list of tools and plugins can be used to manipulate the structures.



A Stash item must be *active* in order to apply an operation by one of the Builder tools.



Once an item is activated, it is visualized in the 3D View. You can also apply operations on a Stash item such as rename, copy, and delete.

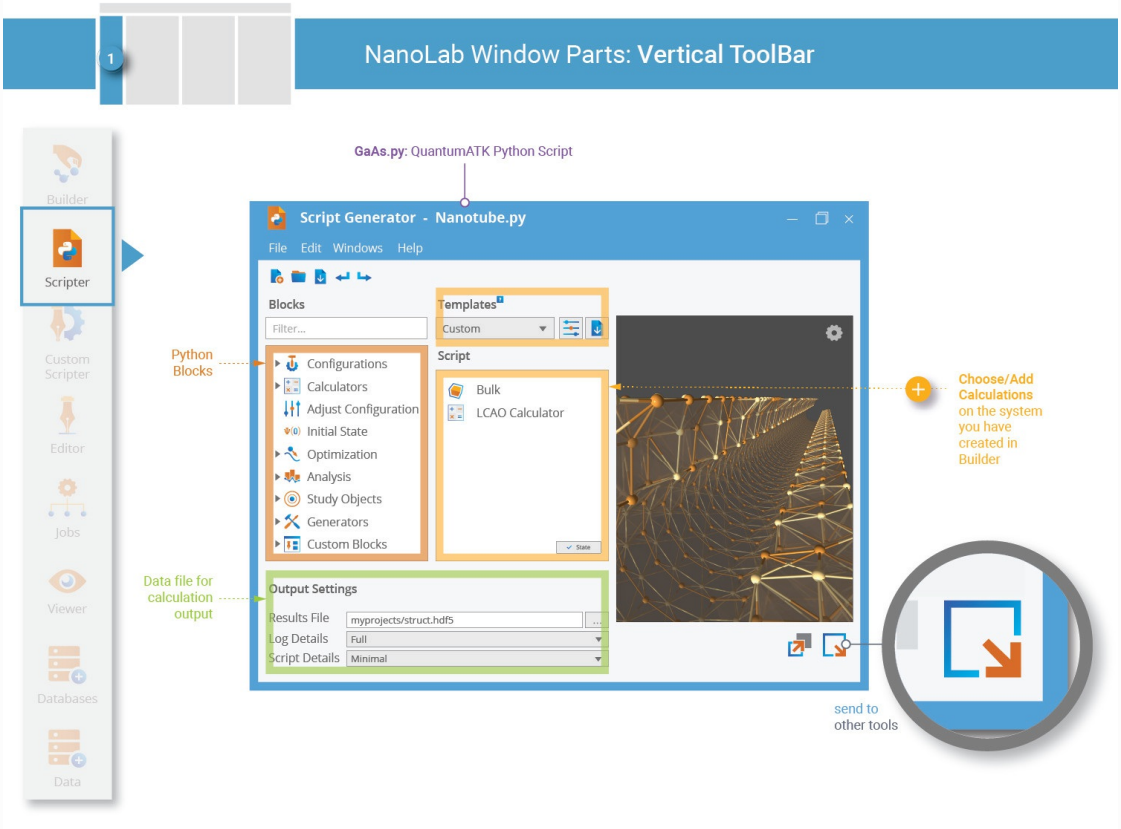


When you have finished building your configuration, use the **Send to** button (located in the lower-right corner of the Builder window) to transfer it to the Script Generator and set up the desired calculations. This is the topic of the next section.

Script Generator

ATK is executed using Python scripting, and the **Script Generator** is a graphical interface for generating QuantumATK Python scripts – it allows you to graphically add blocks of Python code to the script and edit relevant settings if needed.

Simply double-clik a block in the left-hand panel (named **Blocks**) to add it to the **Script** in the right-hand panel. The order of the blocks, from top to bottom, defines the workflow of the QuantumATK calculation.



All data from the QuantumATK calculation is saved in the **Default output file**. It should have file extension `.hdf5`.

Note

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data. HDF5 is portable and is extensible, allowing applications to evolve in their use of HDF5. The HDF5 Technology suite includes tools and applications for managing, manipulating, viewing, and analyzing data in the HDF5 format.

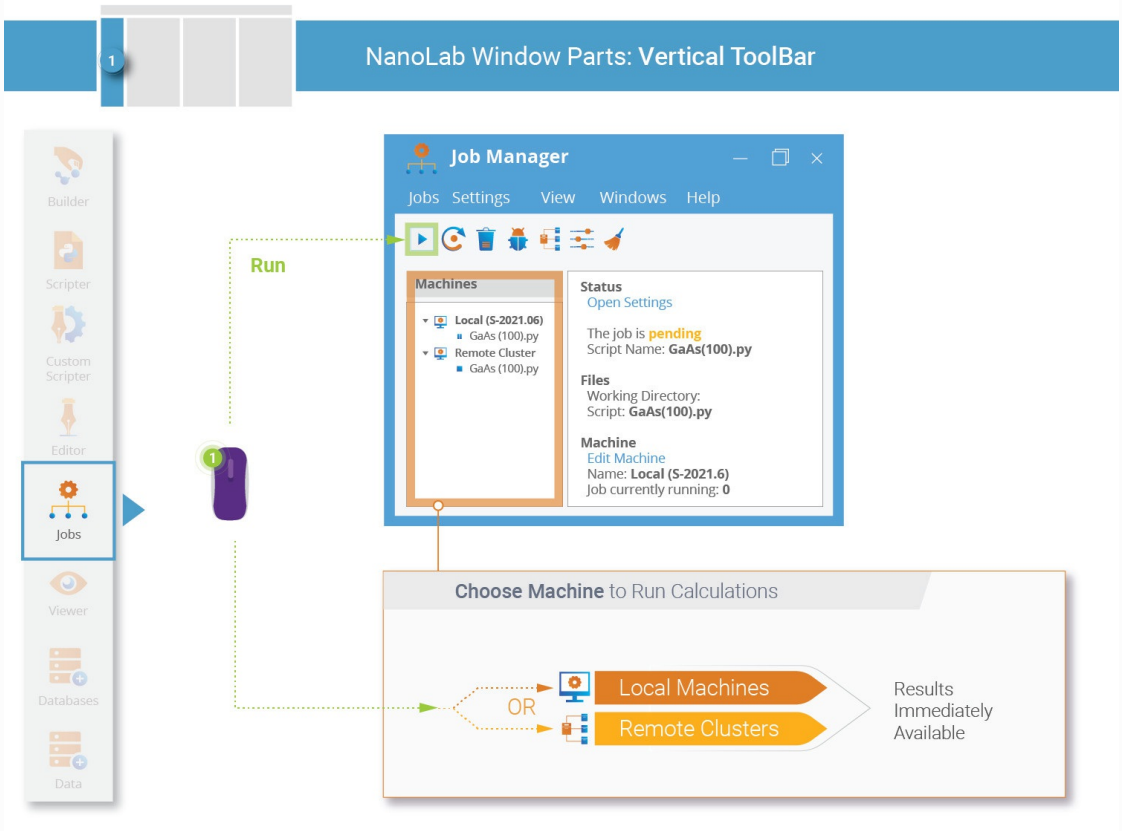
Once you have finished setting up the QuantumATK Python script, you can save it with file extension `.py` and then execute it on a supercomputing cluster or in a terminal on your local machine:

```
atkpython example.py > example.log
```

Alternatively, you can click the button and transfer the script directly to the Job Manager for local or remote execution, see next section.

Job Manager

The **Job Manager** is a graphical interface for executing calculations, both on your local machine and on any remote computing cluster(s) that you have access to.



Once a calculation has finished, the HDF5 data file with results should appear in the **Projects Files** panel in the QuantumATK main window.

Note

The Job Manager allows for parallel execution with MPI and/or threading, see the tutorials Job Manager for local execution of QuantumATK scripts and Job Manager for remote execution of QuantumATK scripts for more information.

Analyzing the Results

Data analysis and visualization is the final step in the most basic QuantumATK workflow: You have built a nanostructure, calculated the electronic structure at some level of theory, and have most likely performed some post-SCF analysis, e.g. computed the electron density and band structure. It is time to visualize the results and perhaps perform further analysis.

The **Project Files** panel shows at all times the contents of the project folder you specified when creating the project (unless filtering is used). This includes QuantumATK scripts (`.py`), QuantumATK data files (`.hdf5`), log files, images, and any other standard file type.

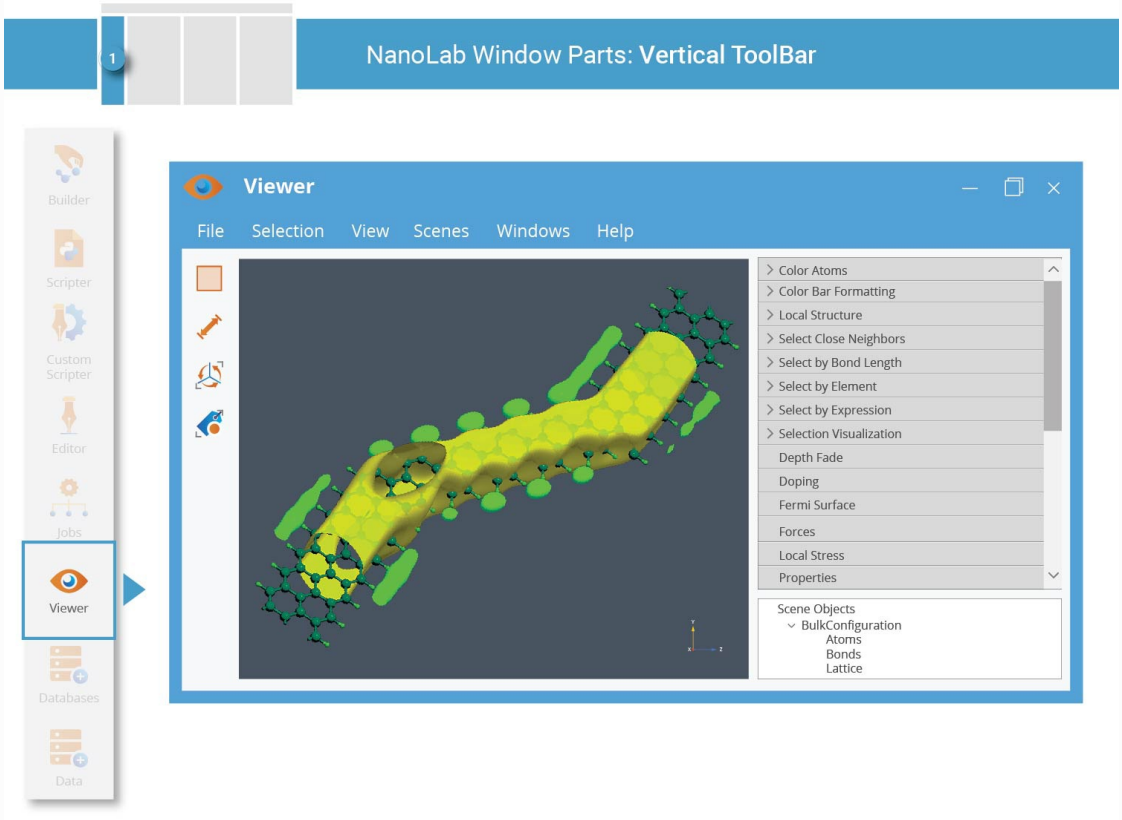
Next, the **LabFloor** shows the contents of the selected (ticked) `.hdf5` data files. QuantumATK reads the data as individual Python *objects*, and displays each object as an easily recognizable *item* on the LabFloor. In the figure below, the data file `GaAs(100).hdf5` contains three saved data items: The band structure, the bulk configuration, and the electron density.

Finally, the **Panel Bar** offers an extensive list of analysis and visualization tools that can be applied to the selected LabFloor item(s). This way, the LabFloor and Panel Bar constitute in total a graphical interface for analyzing and visualizing the data generated by running simulations.

Note

The **LabFloor** will show *all* the objects saved in a `.hdf5` data file, and the contents of newly generated files are automatically added to the LabFloor. Ticking/unticking a file in the **Project Files** list adds/removes its contents from the LabFloor.

A LabFloor item must be *selected* in order to apply an analysis tool to it. Panel Bar tools that cannot be applied to a selected item type are greyed out. The **Viewer** is one possible analysis tool – it is used to visualize configurations as well as grid quantities (e.g. electron density).



Previous Next