



Atomistix ToolKit

Installation guide

Version 12.2.0

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Licensor

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CHAPTER 1. INSTALLATION

INTRODUCTION

This chapter describes how to [install](#) and [start Atomistix ToolKit 12.2.0](#).

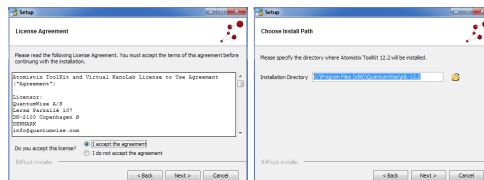
The [next chapter](#) contains information about how to manage [license files](#) and [license servers](#).

It is recommended to [uninstall](#) previous versions of ATK before installing a new version. This is mainly to avoid confusion; two versions can be installed alongside each other without problems, but you will have to take care which version you run.

If you experience any problems during the installation, see the [troubleshooting section](#) for links to useful resources.

INSTALLING ATOMISTIX TOOLKIT

ATK is distributed as a binary installer on both Windows and Linux.



1. [Download](#) the installer for your platform (Windows/Linux, 32- or 64-bit).
2. Double-click the downloaded file, or run it from the command line (on Linux, run it as `./atk-12.2.0-linux64.bin`, or similar for 32-bit, in the directory where you saved the file).
3. Follow the step-by-step instructions to approve the license agreement and choose the installation directory (click "Next" to move to the next step each time).
4. Once the installer finishes, [test the installation](#). If the graphical user interface does not start up normally, please check the sections below, or refer to the [troubleshooting section](#).

Tip

If you are installing ATK on a machine without a graphical interface, e.g. via a terminal window on a cluster, append the option "`--mode text`" to run the installer in text mode. There is also an [unattended mode](#) if you need to deploy ATK on several machines.

LAUNCHING THE PROGRAM

The installer simplifies the process of launching ATK in several ways:

- A shortcut is added to the **Desktop** which you can just double-click to start the graphical user interface, Virtual NanoLab (VNL).
- On **Windows**, shortcuts are also placed in the Start Menu under QuantumWise > Atomistix ToolKit 12.2.0.
- The binary directories for both the command-line interpreter (`atkpython`) and Virtual NanoLab (`vn1`) are added to the system **PATH**, so that you can issue the commands from anywhere on your system.

To verify that the software has been properly installed, and the license is correctly configured, start VNL e.g. by double-clicking the **Desktop** icon.

Note

On **Linux**, you may need to log out and back in again before the desktop icon will work. Also, before you can start ATK from the command line, after the installation, you need to open a new terminal window, so that the changes to the environment are effectuated.

On **Windows**, you should allow ATK and VNL to access the network.

Tip

You execute a Python script with ATK like this:

```
atkpython script.py > logfile.log
```

If, however, you start `atkpython` without any command line argument, you will enter **interactive mode** where you can issue commands directly on the command line (like, for instance, in Matlab). Press **Ctrl+D** to quit.

UNINSTALLING ATK

To uninstall ATK on **Linux**, run the binary `uninstall` in the installation directory.

On **Windows**, ATK can be uninstalled via the Control Panel or by launching the uninstaller from the Start Menu, under QuantumWise > Atomistix ToolKit 12.2.0 > Utilities.

If you have installed the separate **license server package**, follow the same procedure for it, unless you plan to install a new version of ATK - in that case just leave the license server running.

TROUBLESHOOTING INSTALLATION PROBLEMS

If you experience any problems during the installation, first search the [User Forum](#) and/or the [FAQ](#) to see if a solution is posted there. If not, please contact [QuantumWise support](#).

CHAPTER 2. LICENSING

INTRODUCTION

ATK uses the **LM-X License Manager** from [X-Formation](#) to ensure that the usage of the program complies with the terms in the license agreement. In this chapter, you can find basic information about LM-X regarding the points which are most relevant for the operation of ATK. For more detailed information, please refer to the [LM-X End Users Guide](#).

Note

You can try ATK for a time-limited demo period without any license file. The information in this chapter primarily applies to the case where you have an actual license file (a purchased license, a prolonged trial license, etc).

To run ATK beyond the demo period, you must have a license file, and each computer that runs ATK (a "client") needs to be configured properly.

If you:

- **Need a trial license file:** Please contact QuantumWise via the form available from [QuantumWise web site](#) ("Trial license" option).
- **Have a trial license file** (or another standalone license file): See the instructions for [configuring the client](#) to allow ATK to locate the license file.
- **Have a floating license file** (typically the case for a **purchased** license): See the instructions for [configuring the license server](#).

Tip

If you are not sure whether your license file is floating or standalone, ask your QuantumWise contact person, or have a look inside the file itself (it's just a text file). If it contains lines with the keyword "COUNT", it is most likely a floating license.

CONFIGURING A LICENSE SERVER

Running ATK via a license server by using a **floating license** is very convenient, as it makes it possible to run the software on any machine on the network with minimal configuration of the clients.

PREPARATIONS

Before you can set up the license server, there are two steps of preparation:

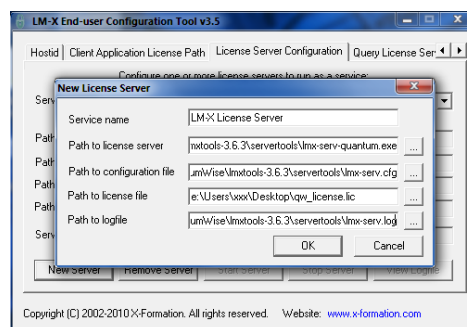
1. Download the **license server package** for the relevant platform, and install it on the license server.
2. Determine the **host ID** of the license server and provide this information to QuantumWise in order to obtain a floating license file.

The following sections describe how to set up the license server on [Windows](#) and [Linux](#).

WINDOWS

Follow these steps to install the LM-X license server as a service on Windows.

1. Start the **License Server Tool** via the shortcut in the Start Menu under QuantumWise > ATK License Server. You can also run `lmxconfigtool.exe` from the command line.
2. When the tool starts up, open the tab "License Server Configuration" and click "New Server". In the dialog box that appears, give the service a suitable name (the default works fine). Then, for each of the four fields, click the "..." buttons to specify the location of the four different files:
 - The license server binary (`lmx-serv-quantum.exe`)
 - The configuration file (`lmx-serv.cfg`)
 - The license file (which you should have received from QuantumWise)
 - The log file (choose a suitable name for the file, like `license_server.log`).The first two files can be found in the same directory as the license server tool itself (i.e. in the `license` subdirectory of the installation directory for the license tool package). It is also recommended to place the log file here.



3. Click "OK" to save the server configuration.
4. Start the license server by clicking "Start server". If successful, you should see the message "Service is running" under "Service status".

Important

If you are asked if the license name server should be allowed to access the network, you must agree.



Note

- The configuration file can be edited to define the port used for license communications and other options, as discussed in an [Appendix](#).
- If you need to update the license file, first stop the server, then replace the license file, and then start the server again.
- To remove the license server, first stop it, then click "Remove Server".

LINUX

TESTING THE LICENSE SERVER SETUP

To test that things work properly, first start the license server in the foreground, from the command line.

1. Run, in a terminal window,

```
lmx-serv-quantum -l licensefile.lic
```

The license file can be located anywhere, as long as you specify it with full path.

The license server should start up with a message similar to the one below.

```
LM-X License Server v3.6 (Linux_x86)
Copyright (C) 2002-2011 X-Formation. All rights reserved.

[2010-05-28 09:53:43] LM-X License Server v3.6.3 build 1234 on localhost (Linux_x86)

[2010-05-28 09:53:43] Copyright (C) 2002-2011 X-Formation. All rights reserved.
[2010-05-28 09:53:43] Website: http://www.lm-x.com http://www.x-formation.com
[2010-05-28 09:53:43] License server has pid 6484.
[2010-05-28 09:53:43] Serving licenses for QUANTUM.
[2010-05-28 09:53:43]
[2010-05-28 09:53:43] License server using TCP IPv4 port 6200.
[2010-05-28 09:53:43] License server using TCP IPv6 port 6200.
[2010-05-28 09:53:43] License server using UDP IPv4 port 6200.
[2010-05-28 09:53:43] Reading licenses...
[2010-05-28 09:53:43] License file(s):
[2010-05-28 09:53:43] /home/user/license.lic
[2010-05-28 09:53:45] Serving following features:
[2010-05-28 09:53:45] atkpython (v12.2) (10 license(s)) license type: exclusive
[2010-05-28 09:53:45]
[2010-05-28 09:53:45] Log file path: Not set
[2010-05-28 09:53:45] Configuration file path: Not set
[2010-05-28 09:53:45] Minimum user remove time set to 120 seconds.
[2010-05-28 09:53:45] Ready to serve...
```

2. If all looks fine (i.e. there are no error messages and you see the daemon "serving" the relevant features), you should check that the license server can be reached from the client computers. A convenient way to do this is to run

```
lmxendutil -licstat
```

on the clients. If the client can reach the license server, it will print information about the server and the license usage:

```
+++++
LM-X License Server on 6200@192.168.0.17:

Server version: v3.6.3 Uptime: 0 hour(s) 5 min(s) 18 sec(s)
-----
Feature: atkpython Version: 12.2 Vendor: QUANTUM
Start date: NONE Expire date: 2012-12-31
Key type: EXCLUSIVE

0 of 1 license(s) used
```

You should also see a few messages on the license server about the client request.

Important

If the client is unable to automatically connect to the license server, the most likely reason is that the communication is blocked by firewall rules. To resolve this, **open port number 6200 (TCP and UDP) in the firewall**, both on the server and the clients, and possibly (but less likely) on any router or hardware firewall in between them.

INSTALLING THE LICENSE SERVER PERMANENTLY

It is convenient to have the license server start up automatically each time the server is rebooted, running as a background process or service.

Before proceeding, close down the license server by pressing **Ctrl-C** in the terminal window where it is running.

To run the license server in the background (for the current session only), you can use the command

```
lmserv-quantum -b -l /path/to/licensefile.lic -lf /opt/logs/lmsserver.log
```

Note

- Use a log file (option **-lf**) to record any error messages from the server.
- All file names (like license file and log file) must be specified with **absolute path**.

To configure the server to start up automatically on reboot, you can use the startup script `lmserv-run.sh` enclosed in the `license` directory. Edit it to reflect your local conditions (like the path to the files, the user account that will run the server, etc), and install it in `/etc/init.d` (or the similar location relevant for your Linux distribution).

Important

- The exact details of start-up scripts, and where to install them, can differ between different Linux distributions. If the provided script doesn't work on your system, please consult your system administration guide.
- The startup script refers to a [configuration file](#); make sure that this file exists in the specified location, and that you have configured it properly.
- If you change the password to the server in the startup script (which is a good idea!), remember to change it also in the configuration file.

-
- Do not run the license server as root! Also note that the user account that runs the service must have a writable home directory (shell access is however not required).

Host ID

Except for trial licenses, all ATK licenses are locked to a particular machine. There are two basic types of licenses:

- **Node-locked license:** The license is tied to a particular machine. ATK can then only run on this computer.
- **Floating license:** The license is tied to the machine hosting the license server. The software can run on any computer that can check out a license from the license server.

The host ID is really just the **MAC address** of the primary network interface of the machine. A few convenient utilities for extracting the host ID are installed with ATK, and also with the separate [license server package](#). You could however just use the operating system functionality to extract the MAC address.

- **Command-line approach:**

Run `lmxendutil` in a terminal window. To save the output, you can pipe it to a file:

```
lmxendutil -hostid > hostids.txt
```

- **GUI tool:**

Start the **ATK License Configuration Tool** via the Start Menu under QuantumWise > Atom-istix ToolKit 12.2.0 > Utilities or (on Linux, but also on Windows) from the command line as `atk_license_config`.

On the first screen which appears you will see all the host IDs of the system.

The host IDs thus obtained should be provided to QuantumWise, so that a license can be issued. You may remove any information you prefer not to share, but you must at least leave the ETHERNET specification of the LAN card (binding to a wireless network interface is discouraged, since it means ATK may not run if the wireless adapter is disabled).

CLIENT SIDE LICENSE MANAGEMENT

Each client that will run ATK needs to be configured for licensing, whether using a [license server](#) or a standalone/node-locked license.

The license configuration can be managed in two ways:

- Via the [interactive license configuration tool](#) provided with ATK. This is the recommended approach for most users.
- By [manually editing the environment variables which control the license configuration](#). This requires that you are familiar with editing environment variables.

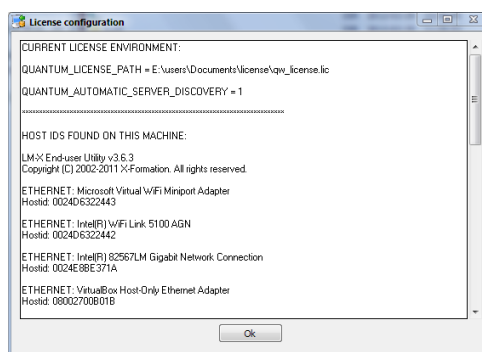
CONFIGURING THE LICENSE INTERACTIVELY

To start the interactive license configuration tool, on a machine where ATK has been installed, you may type

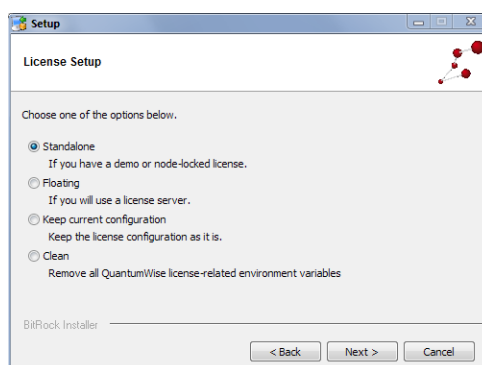
```
atk_license_config
```

on the command line, or (on Windows) use the shortcut **ATK License Configuration Tool** in Start Menu under QuantumWise > Atomistix ToolKit 12.2.0 > Utilities.

The tool provides easy to follow step-by-step instructions for configuring the license environment. On the first page (after the startup screen), the tool will display the current license configuration, along with the host IDs of the machine. This can be helpful when troubleshooting license problems.



On the second page, you will be asked which type of license you have, standalone or floating. The tool can also be used to remove all license environment variables.



- If you choose **standalone**, you will be asked for the location of the license file on the next page.
- If you choose **floating**, you can on the next page optionally specify the location of the license server. Leave this field empty, unless you have already verified that the license server cannot be discovered automatically.

If for some reason the automatic discovery does not work, enter the hostname (or IP address) of the license server, for example `licserv.mydomain.edu`. Do **not** include the port number; if you also have [changed the port](#), you will need to [edit the environment variable manually](#).



Note

The license configuration is in reality controlled by environment variables, as described in the [following section](#). The interactive tool is just a convenient way to edit these variables.

LICENSE CONFIGURATION VIA ENVIRONMENT VARIABLES

This section documents how the ATK license configuration is controlled by environment variables. If you are familiar with editing system and user environment variables, you can directly modify the license configuration by setting the variables to their desired values. In many cases, it is however easier and safer to use the interactive license configuration tool described in the [previous section](#).

The license configuration is controlled by two environment variables:

- **QUANTUM_AUTOMATIC_SERVER_DISCOVERY**

By setting this variable to 1, ATK will be able to automatically detect a license server over the network. In this case there is no need to set **QUANTUM_LICENSE_PATH**, and no additional configuration is typically needed on the client, except you may need to [open the relevant ports](#), if software or hardware firewall rules prevent the automatic server detection.

The ATK installer will always set this variable to 1; thus, no additional client configuration is actually needed to use a floating license server.

- **QUANTUM_LICENSE_PATH**

- For standalone licenses (node-locked or demo/trial licenses), this variable should point to the complete, absolute name of the license file, or a directory in which to look for license files (files with extension `.lic`).
- In the unusual case that automatic server discovery does not work, this variable can alternatively be used to define the license server manually. In this case, set the variable to the hostname/IP address of the license server, using the following format:

```
[port]@hostname
```

where the **port** specification is optional and only needed if your server uses a different port than 6200.



Important

The "@" sign is *required*, even when using the default port!

NOTES

For definiteness it is assumed below that your Linux shell is `bash`. The corresponding changes for `tcsh` and other less common shells should be obvious to experienced Linux users.

- Network license servers have priority over local license files. Therefore, to switch from using a floating license server to a node-locked license file (e.g. if you receive a temporary, node-locked or demo license) you must unset the environment variable **QUANTUM_AUTOMATIC_SERVER_DISCOVERY**. Note that this variable is automatically set to **1** by the installer.

-
- You can specify multiple servers and/or files/directories by separating them with a semicolon ";" (on Windows) or colon ":" (on Linux).

Example (Linux):

```
export QUANTUM_LICENSE_PATH=@server.abc.com:/home/user/licenses:@backupserver.abc.com
```

- On Linux, the installer defines the license environment variables to two separate files in your home directory:
 - `.profile` (or possibly `.bash_profile`). This file defines the environment for the Desktop, but is not read if you connect via ssh for instance.
 - `.bashrc`. This file defines the environment for all terminal windows, and is read also on ssh login.

If you modify the license setup manually, it is recommended to remove the ATK environment variables from `.profile` and only define them in `.bashrc`, to avoid confusion. `.profile` normally anyway sources `.bashrc`, thus the changes will also apply to the Desktop environment.

Important

To activate changes in `.profile` (including those sourced from `.bashrc`) you must log out and log back in again. This really only affects the VNL desktop icon; changes in `.bashrc` take effect as soon as you open a new terminal window.

CHAPTER 3. APPENDIX

UNATTENDED INSTALLATION

It is possible to run the installer in "unattended" mode. This is useful for automated installations of a network of computers. With this mode, the installer will not prompt the user for any information and will instead take the default settings configured for each of the parameters.

We will symbolically call the installer binary `atk-installer` below; running in unattended mode can only be done from the command line.

To install ATK for a floating license server in unattended mode, run

```
atk-installer --mode unattended --license_configuration floating
```

For standalone licenses (demos and node-locked), make sure the license file resides in the same directory as the installer (for simplicity), and run

```
atk-installer --mode unattended --license_configuration standalone --license_file qw_license.lic
```

Tip

You are not forced to use only the default values when running the installer in this mode. Custom values can be defined through command line switches; for a full list of these, type

```
atk-installer --help
```

For example, to add a progress bar, append the option

```
--unattendedmodeui minimal
```

To specify another installation location than default, use the option **--prefix**.

For more information, see the [BitRock documentation](#).

ADDITIONAL OPTIONS TO THE LICENSE SERVER

There are several additional options that can be used to configure the license server. These options are defined in a so-called **configuration file**, a template for which (`lms-serv.cfg`) is included with the license server files.

For general information about this file and the options you can set in it, please refer to the [LM-X End Users Guide](#).

To invoke the configuration file when you start the license server manually on Linux, use the option `-c`

```
lmx-serv-quantum -b -l licensefile.lic -c lmx-serv.cfg -lf logfile
```

! Important

If you use a startup script on Linux (see [above](#)), the location of the configuration file is defined in the script via an environment variable and not directly on the command line.

On Windows you specify the configuration in the license configuration tool when [defining the service](#).

SPECIFYING THE SERVER PORT

The only two options that are activated (not commented out) in the configuration file included with ATK by default are the port number and the password for the license server.

By default, the license server uses TCP and UDP ports 6200 for communication across the network. The UDP port is hard coded and cannot be changed, but you can specify a different TCP port (e.g. in case there is a conflict with another LM-X license server). To do so, edit the line in the configuration file:

```
TCP_LISTEN_PORT = 6200
```

In this case it is also necessary to explicitly specify the port and hostname of the license server on the clients via the [environment variable](#) `QUANTUM_LICENSE_PATH`.

HIGH-AVAILABILITY LICENSING (HAL)

LM-X offers a so-called high-availability licensing (HAL) scheme, in which three redundant servers are providing the same license. If one server goes down, the two others will still work. This requires a special license file; please contact QuantumWise if you are interested in this option.

The procedure for installing HAL servers is the [same as for a single license server](#), except you do it on all three servers, with the important addition that the [configuration file](#) should contain a list of all HAL servers:

```
HAL_SERVER1 = 6200@server1  
HAL_SERVER2 = 6200@server2  
HAL_SERVER3 = 6200@server3
```

More information about HAL licensing is provided in Chapter 8 of the [LM-X End Users Guide](#).

MONITORING LICENSE USAGE

To find out how many licenses that are checked out at a given time, and by whom, run

```
lmxendutil -licstat
```

On Windows, you can also use the [License Server Tool](#) for this purpose.