



Virtual NanoLab

Installation Guide

Version 2008.10

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Version 2008.10

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Virtual NanoLab License to Use Agreement

Licensor

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CHAPTER 1. VNL INSTALLATION GUIDE

Thank you for choosing Virtual NanoLab from QuantumWise!

Here we will describe how to install and start the program. It will be assumed that you have basic knowledge of how to install programs and manage your operating system.

SYSTEM REQUIREMENTS

VNL currently runs on most **Microsoft Windows** or **Linux** platforms on 32 bit PCs.

More specifically, the following **processors** are supported:

- 32-bit PC architectures
 - *Intel*: Pentium III, Pentium 4, Pentium M, Intel Xeon, Pentium 4 EM64T and Xeon EM64T, etc.
 - *AMD*: Athlon XP, Athlon 64, Opteron, etc.

As for **operating systems**, the following are supported:

- 32-bit Linux (*Detailed requirements apply, which affect compatibility of different distributions*).
- Microsoft Windows 2000, XP, and 2003

For a much more detailed list of system requirements as well as particular information about the compatibility of different Linux distributions, please refer to the [QuantumWise web site](#), where updated information is available.

To install VNL, you need about 330 MB available **storage space** on the installation drive. However, the result files created when running the program can often become large. It is therefore recommended to have at least 500 MB available, but note that certain calculations can require gigabytes of storage space.

The tasks performed in VNL involve complex numerical calculations, which demand a lot of both the computer processor and memory. Although there is no specific minimum requirement, other than those that generally apply for running applications on each specific platform, it is highly recommended to equip the computer with a **large amount of memory** (both RAM and swap), with 512 MB as an absolute minimum, and 1 GB as a reasonable number for larger (but not too large) calculations. As for the **processor**, it is a good idea to have at least a Pentium 4 or correspondingly, and certainly above 2 GHz clock frequency.

INSTALLING THE PROGRAM

Please follow the step-by-step instructions below to install the program. Note that in addition to installing the program itself, it is also necessary to set up a valid **license**.

On both on Linux and Windows, the installation procedure generally consists of four steps

1. Extracting the installation package.
2. Configuring the system environment.
3. Setting up the FLEXlm license system.
4. Run a simple test to check if the installation was successful.

If you experience any problems during the installation or use of the software, please contact [QuantumWise support](#).

LINUX

1. For Linux, the program is distributed as a **bzip2** compressed tar-ball, which must be unpacked in the desired installation directory. If you are installing for a single user, it is probably best to install the program in your own home directory, but you may of course also install it system-wide if you have the relevant permissions.

Copy the tar-ball — here, symbolically named `vn1.tar.bz2` — the exact filename differs for different hardware/operating system configurations) to the directory where you wish to install the program. Open a terminal window and navigate to the location of the tar-file. We will symbolically refer to this directory as `install_dir`; typically, it will be your home directory, but this is not required.

Type and execute the command

```
tar xvfj vn1.tar.bz2
```

at the command prompt. This creates a new sub-directory called `vn1` (if it does not already exist) and extract all program files into it.

2. To simplify starting the program, it is recommended to include the VNL binary directory (`vn1/bin/`) in your **path**, or add a desktop icon pointing to the program.

The exact details for defining the path and creating desktop icons depend on your shell and windows manager; please refer to the associated documentation — some useful hints are also available in the Atomistix ToolKit 2008.10 Installation Guide, which you may download from [QuantumWise web site](#).

3. The final step of the installation procedure is to install the **license**. This is described in [the section called "License"](#) below.

WINDOWS

In this Installation Guide it will be assumed that you are running an English version of Windows XP or Windows 2000, and that Windows is installed with user settings stored under

c:\Documents and Settings

If you are running a different Windows version, using a different interface language, or the location of the Documents and Settings folder is different, it is necessary to modify the installation instructions accordingly.

1. VNL is installed by **double**-clicking the distributed .exe file, and by following the on-screen instructions.

During the installation, you may choose in which **directory** you wish to install the program (C:\Program Files\QuantumWise\Virtual NanoLab 2008.10 being the default), and whether to install it for all users on the computer (this option is only available with **Administrator** privileges), or for yourself only.

2. VNL is launched by using the **shortcut** in the **Start menu** under **Programs** → **QuantumWise** → **Virtual NanoLab 2008.10**. A VNL icon is also installed on the **Desktop**.
3. The final step of the installation procedure is to install the **license**. This is described in [the section called "License"](#).

LICENSE

In order to run VNL you must have a valid **license**. VNL uses the **FLEXlm** license system from [Macrovision](#), which supports many different solutions for managing licenses.

Installing licenses is a rather simple process, and will be covered below by simple step-by-step instructions. In some cases it is however necessary to go into more advanced details regarding the licenses. Detailed information about all possible aspects regarding FLEXlm licenses can be found in the [FLEXlm End User Guide](#) which we recommend users to download and read, should you have any questions regarding FLEXlm licenses. You are of course also welcome to contact [QuantumWise Support](#) if you have any problems.

In general, the following list outlines the steps involved towards obtaining and installing a valid license so that VNL can be run.

1. Decide which license type you require.

Node-locked licenses are **uncounted**, i.e. they support an unlimited number of simultaneous processes, but these processes are limited to run on a particular computer with a single CPU.

Floating licenses are **counted**, i.e. there is a limitation to the number of processes that can run concurrently. On the other hand, these processes can be launched on any computer in your network that has access to the license server managing the floating license, or on a multi-CPU machine.

In a network situation, the license of choice is clearly floating, if you want all computers on the network to be able to run the software.

For a single computer, you have to distinguish between two cases. If the computer is equipped with more than one CPU, it is necessary to have a **counted floating license** corresponding to the number of CPUs; if your computer only has a single CPU, it is sufficient to obtain an **uncounted node-locked license**.

In other words, several considerations must be taken into account when deciding on the type of license to purchase. For advice and more information about license types and prices, please contact QuantumWise or your local distributor.

2. The licenses for VNL are **always** issued for a specific **host computer**, both in the case of node-locked and floating licenses. In order to obtain a license file for your system, it is therefore necessary to provide the **FLEXlm host ID** of the license host computer to QuantumWise.

The detailed procedure for determining the host ID is described in [the section called “How to Determine the Host ID”](#).

3. Once you have obtained the required information, send it by email to QuantumWise (sales@quantumwise.com), together with your **Customer ID** and other identifying information. Your license file will then be returned to you by email.
4. **Install** and test the license file, as described in the subsequent sections.

The detailed steps for installing the license file are somewhat different for Linux and Windows, and again different depending on if you will be using a **license server** or not. A license server is always required for [floating licenses](#). For [uncounted node-locked licenses](#), however, the license file is sufficient by itself.

HOW TO DETERMINE THE HOST ID

For a node-locked license, the host ID refers to the computer where you will run VNL, whereas for a floating license the host ID should correspond to the license server.

In either case, the host ID is nothing but the MAC address of your network card. This address can be extracted from your system in many different ways, but FLEXlm provides a simple utility to extract the address, and this utility is shipped with the VNL package.

On **Linux**, navigate to the `bin` directory under the VNL installation directory and run

```
./lmhostid
```

If you included the VNL binary directory in your path, you can execute this command from anywhere.

On **Windows**, the utility is installed as a shortcut called `lmhostid` in the [Start menu](#) under [Programs](#) → [QuantumWise](#) → [Virtual NanoLab 2008.10](#).

Running the FLEXlm utility will, on either platform, produce a message:

```
The FLEXlm host ID of this machine is "01030e10b1b9"
```

The numbers enclosed in quotation marks is unique for any computer; this is the host ID. Note that if you have more than one network card in your computer, there will be several lines with different host IDs. Please include all of them in the email you send to QuantumWise.

UNCOUNTED NODE-LOCKED LICENSE

An uncounted node-locked license can only be used on the host specified in the license file. It can not be used for parallel computations, and does not require the installation of a license server. An uncounted license can not be used on a computer with more than one CPU.

LINUX: UNCOUNTED NODE-LOCKED LICENSE

FLEXlm stores the information about licenses in a text file called `.flexlmrc` in the user's home directory (note the initial dot). This file contains the line

```
VENDOR_LICENSE_FILE=/path/to/file/licensefile.lic
```

for each installed license. It is possible to have several licenses defined in the `.flexlmrc` file simultaneously, and if you are running other applications such as MATLAB or Maple, you may already have this file in your home directory. QuantumWise's licenses are identified by lines starting with our vendor id `ATOMIST`.

In order to install, remove, or deactivate licenses, it is possible to edit this file. Otherwise, go through the following **step-by-step instructions** to install your license file.

1. First of all, it is recommended to **uninstall** all older FLEXlm licenses from QuantumWise first. The latest license file received from QuantumWise always contains all purchased valid licenses, so there is no need to retain older license files.

To uninstall all QuantumWise licenses, edit the `.flexlmrc` file and remove the line starting with `ATOMIST`. If you have no other applications on your system that use FLEXlm, you may delete this file.

A safe way to remove all references to QuantumWise licenses in the `.flexlmrc` file is to run the script `flexlm_cleanup.sh` provided in the same directory as the VNL binary.

2. Place the license file in a suitable location, preferably in sub-directory of the VNL installation directory. If you place the license file there, you may proceed directly to this [step](#).
3. If you place the license file anywhere else than the one stated in the previous step, it is necessary to inform FLEXlm of its location. In a terminal window, type the command

```
export ATOMIST_LICENSE_FILE=/path/to/file/license.lic
```

where `/path/to/lic` symbolically denotes the full path of the license file. Also make sure to verify the **name** of the license file; normally it is always `license.lic` but it is best to double-check.

4. If you included the VNL binary directory in your `PATH` (see [step 2](#) above), launch the program from a terminal window by executing the command

```
vnl
```

If the program starts normally, then the installation of the license file has been successful.

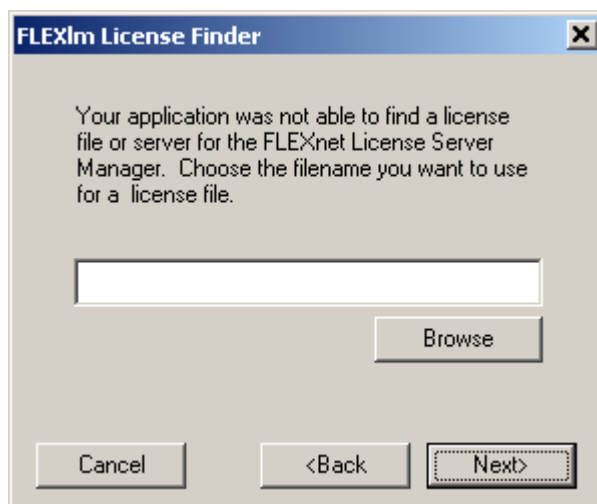
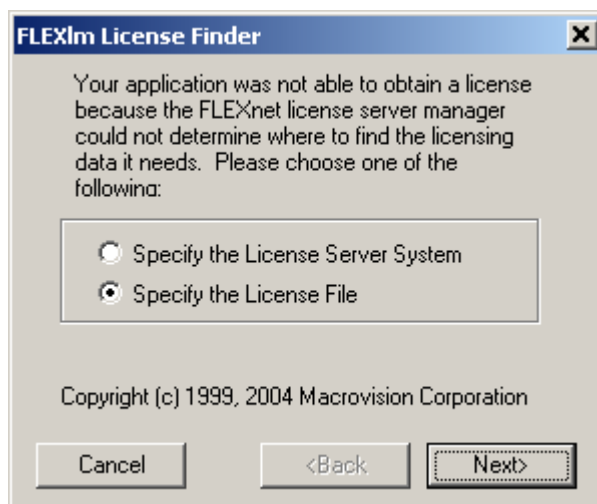
If you, for some reason, chose not to update your path, you obviously have to provide the complete path to the VNL binary.

5. The information about the license file should now automatically have been entered in the FLEXlm resource file, and the installation of the license file is **completed!**

WINDOWS: UNCOUNTED NODE-LOCKED LICENSE

The instructions that follow assume that you have **Administrator** privileges on your computer. If you do not, it is still possible to install the license file, but you should then go immediately to this [step](#).

- The easiest way to proceed is to make sure you start with a clean license environment. This can be achieved by running the small registry script `flexlm_cleanup.reg` provided in the VNL distribution in the same directory as the VNL binary. **Double**-click this file, and click **Yes** in the dialog window that pops up, and then **OK**.
- Place the license file in a suitable location. This can really be anywhere on your system, but make sure to place it in a location where you can easily find it again.
- The simplest way to install the license file is to launch VNL from the Start menu shortcut `Programs → QuantumWise → Virtual NanoLab 2008.10`.



The program will now prompt for the location of the license file (see the above figure). Select **Specify the License File** and click **Next**. On the next screen, type in the full name (including the path) of the license file, or simply click **Browse** to locate it interactively. Once the license file has been specified, click **Next**; if the license file was accepted, a message appears saying “The FLEXnet license finder has completed”. Click the **Finish** button.

After completing these steps, the information about the location of the license file is stored in the Windows Registry in the key `ATOMIST_LICENSE_FILE` under

```
My Computer\HKEY_LOCAL_MACHINE\SOFTWARE\FLEXlm License Manager
```

- When installing as a **restricted user** (i.e. without Administrator rights), the license file cannot be set up automatically or using the FLEXlm utilities. Instead, it is necessary to install the license file manually through an **environment variable**. The following steps describe how to do this on a Windows 2000/XP system:
 - Start the **Control Panel** from the Start menu entry [Settings](#), and open the **System** tool.
 - Open the **Advanced** tab, and click the button **Environment variables**.
 - Click **New...** in the upper panel (under user variables), and in the dialog that appears enter `ATOMIST_LICENSE_FILE` under **Variable name**, and under **Variable value** type the complete file name (including the path) of the **license file**.
 - Click **OK** and close all opened windows.

This procedure can also be used even if you are Administrator, if you prefer to store the license information in the environment variable rather than in the Windows Registry.

LICENSE SERVER

When using QuantumWise software with FLEXlm floating license, the license file specifies the number of VNL processes that can run simultaneously, and also how many nodes that can be used for a parallel calculation. The license is not tied to any specific node, but a specific machine in the network is chosen to serve as **license server**, and will run the FLEXlm license manager software **lmgrd** which handles the license management. In a floating license environment, the license control is centralized to one license server machine in the network. Hence all machines where VNL is installed must be connected to the same network by TCP/IP in order to run.

There are two separate tasks involved in setting up floating licenses:

- setting up the **license server**
- configuring the **clients**

First, make sure to download all the required files:

- The license file (`license.lic`).
- The vendor daemon (**atomist**).
- The license manager (**lmgrd**).

The two latter are **platform-dependent binaries**, whereas the license file is a text file.

The **license file** will be sent to you by email from QuantumWise, once you have provided the required information (see [above](#)), whereas the **vendor daemon** can be obtained from [the QuantumWise download area](#).

The user name and password credentials are the same as when downloading the software package itself. Make sure to download the **atomist** binary for the relevant **architecture** of your license server.

Finally, the **license manager lmgrd** should be downloaded directly from [Macrovision](#).

Make sure to download the binary for the relevant **architecture** of your **license server**; it is also recommended to download the utility **lmutil** from the same location. The files for Linux/UNIX platforms are Z-compressed, which can be decompressed using the **uncompress** or **gunzip** commands.

Windows users should also download the end user utility (a graphical user interface program) called **lmtools**.

Note that it is **not** necessary to download or install any of these three files on the clients that will run VNL, but only on the **license server**.

LINUX: LICENSE SERVER

We will first describe how to **start the license server manager manually**, and then give an example of how it can be set up to start automatically at system start-up.

- Installing the license server
 1. It is recommended to place all the relevant files in the same directory on the license server. For further instructions on how to specify individual paths to the different files, please refer to the [FLEXlm End User Guide](#).
 2. For security reasons, the user that launches **lmgrd** must **not** be **root**, but instead a restricted user should be used.

Ensure that the daemons **lmgrd** and **atomist** have the relevant **permissions** for the user that will launch **lmgrd**, and that they are both **executable**. This can be achieved by the commands

```
chown <user> atomist lmgrd
chmod +x atomist lmgrd
```

These commands must be given in the directory where the files are located, and the first command should be given by the user that currently owns the files (or by root), and **<user>** should be replaced by the relevant user name.

3. To start the license server manually, use the following command:

```
./lmgrd -c license.lic -l log &
```

where the second (optional) option specifies where to store the log message.

In fact, here it is possible to provide the full **path of the license file**, if it is not located in the same directory as **lmgrd**. The vendor daemon **atomist** must however still be located in the same directory as **lmgrd**, unless you modify your license file (see [below](#)).

If the installation is successful, the log may look like:

```
12:11:37 (lmgrd) License file(s): license.lic
12:11:37 (lmgrd) lmgrd tcp-port 27001
12:11:37 (lmgrd) Starting vendor daemons ...
12:11:37 (lmgrd) Started atomist (internet tcp_port 40372 pid 4752)
12:11:37 (atomist) FLEXnet Licensing version 10.1.3
12:11:37 (atomist) lmgrd version 10.8, atomist version 10.1
12:11:37 (atomist) Server started on localdomain for: f1
```

- **Configuring the clients**

The final step is to configure the **clients** to use the floating license server. The procedure is basically identical to setting up a node-locked license, as described above, and the only difference is that instead of a license file, you should specify the **port** and **host name** of the

license server. The default port is 27000 (although this can be changed freely in the license file by the user), so a typical setup would be to replace the [step](#) in that process by

```
export ATOMIST_LICENSE_FILE=27000@licensehost
```

where `licensehost` is the host name (or IP number) of the floating license server.

After that, simply launch VNL, and the relevant information will automatically be entered in the `.flexlmrc` file, and the license setup should be **complete!**

- **Automatic start-up of lmgrd on Linux**

If you want **lmgrd** to start automatically at boot up, you may write a script and put it in `/etc/init.d`. Please consult your system administrator on how to write one, or use the sample script called `flexlm_atomistix.rc` (provided in the same directory as the VNL binary) as a template, and install it as a system service by

```
chkconfig --add flexlm_atomistix.rc
```

Before attempting to install this script, it is crucial to check and modify the path to the license file to reflect your local settings.

WINDOWS: LICENSE SERVER

To set up a **floating license server** under Windows is straightforward using the FLEXlm utility **lmtool**. Please refer to the [FLEXlm End User Guide](#) for all details.

On the **clients**, the only difference compared to the [instructions for node-locked licenses](#) is that instead of specifying a license file in the dialog box that appears when one attempts to start VNL (after uninstalling all existing QuantumWise FLEXlm licenses), you should select "Specify the License Server System", and then specify the port and the hostname of the license server, e.g. as

```
27000@licensehost
```

where 27000 is the port number (27000 is the default, but it can be changed freely in the license file) and `licensehost` is the host name (or IP number) of the floating license server.

FORMAT OF THE LICENSE FILES

In this section, we will present some technical details about the format of the license files. More details can be found in the [FLEXlm End User Guide](#).

NODE-LOCKED LICENSE FILE

A generic node-locked license file from QuantumWise has the following general format:

```
FEATURE VNL atomist 1.2 permanent uncounted HOSTID=01030e10b1be \
SIGN="1DFB 3E10 4DDE B571 46B0 5B09 EEC4 0CD6 3C20 6F69 \
2C13 2C5E E6C6 38EE 1911 204D 983B 4D8D B5FF 5489 2D61 \
19EE 2C13 1B91 13A8 4CE6 17C5 89C5 5D3E B6F1"
# Customer id: 000 # License id: 000
```

The order of some of the entries may be slightly different in your license file, and some additional entries may be present, including **comments** (which start with the “#” character).

Each line starting with the word **FEATURE** describes a particular **license feature**, which gives access to certain functionality in the program. Note that the license file in this example effectively only contains three lines, since a backslash “\” at the end of a line is a “continuation” character, meaning that the line in fact is continued on the next. The line breaks are merely introduced to avoid very long lines in the file and to make it more readable.

The **feature name** appears as the second element on each feature line. In the example above, the feature is symbolically called “f1”; in a real QuantumWise license file, you can at present expect to find the following features:

- **f1** : ATK 2.0 alpha and beta version demo license, or license for running.
- **f2** : Virtual NanoLab 1.1 license.
- **ATKmaster** : Master license for ATK.
- **ATKslave** : Slave license for running ATK in parallel.
- **VNL** : Virtual NanoLab 1.2 license.

The third entry on each feature line is the the so-called **vendor ID**; it will always be **atomist** for licenses from QuantumWise.

The fourth entry is the **version number** of the license feature.

The fifth entry is the **expiration date** of the license, or the word **permanent** if the license is proprietary (i.e. never expires).

The sixth entry is the **number of licenses** issued for this feature. For an uncounted node-locked license, this entry will be **uncounted**.

The final entry on each line is the **host ID** of the computer where this license is valid. As pointed out earlier, it is simply the network card address of that computer.

The final entry, **SIGN**, is the license key itself.

A node-locked file may not be modified in any way, or it will cease to work. The only exception is that you may include comments (starting with #) and spaces and line breaks (remembering to include appropriate continuation characters) to improve the readability.

FLOATING LICENSE FILE

A typical floating license file from QuantumWise has the following general format:

```
SERVER license.server 1a3a3e4b89ed 27000
VENDOR atomist
FEATURE ATKmaster atomist 2.0 8-mar-2016 10 ISSUED=8-feb-2006 \
SIGN="052A 68C5 C679 7E17 012E 9EA9 447C CCFB \
4EEA 9A40 68DF 0707 BEEB E9AB B5DB 0B66 6E2E 2E12 2303 \
D943 506B 05DA 21B1 FDE2 6D13 5EDF F55A 56B2 AFDE 69E8"
FEATURE VNL atomist 1.2 8-mar-2016 100 ISSUED=8-feb-2006 \
SIGN="052A 68C5 C679 7E17 012E 9EA9 447C CCFB \
4EEA 9A40 68DF 0707 BEEB E9AB B5DB 0B66 6E2E 2E12 2303 \
D943 506B 05DA 21B1 FDE2 6D13 5EDF F55A 56B2 AFDE 69E8"
# Customer id: 000 # License id: 000
```

The **FEATURE** blocks in the floating license files are identical to those that appear in the node-locked license files, except that they do not contain any reference to any host id — this is what makes the license floating. It is possible to mix floating and node-locked features in the same license file, if needed.

The first line contains information about the license server. The second entry on the first line is the **host name** of the license server; this name can be freely changed, if needed. The third entry on the first line is the **host ID** of the license server, and the final entry is the **port** that will be used for the license daemon. The default value is **27000**, but this may also be modified to suit local conditions.

The **VENDOR** line specifies the name of the vendor daemon, which is always **atomist** for QuantumWise licenses. If you need to place the vendor daemon in a different directory than where the **lmgrd** daemon is located, it is possible to modify this line by adding the full path (including the name of the vendor daemon) as a **third argument**. As an example, assuming that the daemon binary **atomist** is placed in `/opt/quantumwise/license`, the second line should be modified to read

```
VENDOR atomist /opt/quantumwise/license/atomist
```

As with the node-locked license file, no other parts of the file should be modified, or the license file will most likely cease to function.

UNINSTALLING

To uninstall VNL under **Linux**, simply remove the entire directory into which the program distribution was extracted.

Under **Windows**, the program is uninstalled via **Add and Remove Programs** in the **Control Panel**, or by starting the installation program again and choosing the remove/uninstall option. VNL does not install any files outside its own installation directory.

SUPPORT

Please make sure that you follow the instructions and steps described above closely. Unless you are very familiar with the FLEXlm license format, we recommend that you do not modify your license file in any way; if you do, it can not be expected to work properly.

If you have any trouble installing **licenses**, we recommend that you first have a look at the [FLEXlm End User Guide](#), which provides a lot of details.

You are of course welcome to contact QuantumWise support via the [Help Desk](#) if you experience any problems installing or running VNL.

In addition, you may also find some general advice about VNL on the [QuantumWise web page](#) under **Support**.

We hope that you will enjoy working with VNL!

The QuantumWise Team, December, 2008

