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2. Installation

2.1. Overview

This chapter documents the procedures for installing *Virtual Reactor* and its license server, the Reprise License Manager (RLM). The following steps lead you through the process of getting started with *Virtual Reactor*:

1. [Create a CPFD Support site account](#) in order to access downloads
2. Acquire hardware that meets recommended [System Requirements](#)
3. [Plan the Client-Server Configuration](#)
4. [Download Virtual Reactor](#)
5. [Install the RLM Server](#)
6. [Install the RLM License](#)
7. [Install Virtual Reactor](#)
8. [Point Client Machines to the RLM Server](#)
9. [Install NVIDIA Drivers](#)

In order to use *Virtual Reactor*, you must have a valid software license installed. *Virtual Reactor* uses a client-server model for licensing, meaning that your license(s) can be placed on one machine, which acts as a license server, and other machines on the same network can point to and request licenses from that server. The server may also use the license(s) that it hosts.

The licensing policy for *Virtual Reactor* is as follows:

- Each solver license allows the user to run one instance of the *Virtual Reactor* solver. Optionally, add-ons to each solver license may be purchased to include Chemistry capabilities and/or Parallel capabilities.
- The number of *Virtual Reactor* solvers that can be run simultaneously is limited to the number of solver licenses that have been purchased.
- With any license, an unlimited number of *Virtual Reactor* Graphical User Interfaces (GUIs) can be open at the same time. This allows users to set up simulations, review previously set up models, and use all functions of the GUI.
- [Running a single time step](#) does not count against the number of *Virtual Reactor* solver licenses in use. This allows users to review a project setup at any time.
- An unlimited number of GMV post-processing instances can be open at the same time.
- If Parallel add-on licenses have been purchased, *Virtual Reactor* can utilize NVIDIA GPU cards to increase calculation speed. The number of simulations that can use GPU acceleration simultaneously is limited to the number of Parallel add-on licenses purchased.
- If Chemistry add-on licenses have been purchased, *Virtual Reactor* can include user-specified chemical reactions in the simulation. The number of simulations that can solve chemistry simultaneously is limited to the number of chemistry add-on licenses that have been purchased.
- If Parallel and Chemistry add-on licenses have been purchased, *Virtual Reactor* can use multiple CPU cores for parallelization of volume-average chemistry to increase calculation speed. The number of simulations that can use CPU parallel acceleration simultaneously is limited to the number of Parallel add-on licenses purchased.

2.2. System Requirements

Virtual Reactor can be used on either Linux or Windows. The following table lists minimum and recommended system requirements.

Minimum	Recommended
---------	-------------

	Minimum	Recommended
Operating System	Recent 64-bit Linux 64-bit Windows 7, 8, or 10	64-bit CentOS 6 (RHEL 6) or higher Windows 7 Professional 64-bit
CPU	Any 64-bit Intel compatible from the last 5 years	Intel Core i7-4790K or better i7/Xeon. Higher clock speed, and newer Intel architecture are better.
Memory (RAM)	8 GB	32 GB or more. Faster is better.
Hard drive space	500 GB	8 TB (2x 4TB) or more
GPU *	NVIDIA GPU required	NVIDIA GeForce GTX Titan X (Pascal)
CUDA Compute Compatibility *	2.0	3.5 or higher
GPU RAM *	4 GB	12 GB or more

* - GPU requirements only apply if *Virtual Reactor* will be running in GPU parallel mode. The required GPU RAM is also dependent on the size of the simulation being run. A larger simulation will require more GPU RAM.

Though *Virtual Reactor* simulations can be run on laptops, or lower-performance desktop machines, doing so is generally not recommended. Investing in an up-to-date calculation machine, with the fastest hardware currently available, will provide much faster calculation speeds. Additionally, since computer hardware advances in capacity and speed at such a fast pace, it is recommended to purchase updated hardware every 2 to 3 years to obtain the fastest performance.

Virtual Reactor can be installed on compute nodes of a cluster. However, it will not take advantage of the multi-node parallel computing capabilities of the cluster. Each *Virtual Reactor* simulation utilizes the computing resources of a single machine. Parallelization is available through the use of an NVIDIA GPU, or through CPU-parallel solution of volume-average chemistry. Since each individual node of a cluster is not usually optimized for the fastest possible single-machine CPU performance, it is often the case that running *Virtual Reactor* on a cluster node will not give the best possible calculation speed. Instead, it is generally better to purchase a very fast single-CPU standalone calculation machine on which to run *Virtual Reactor*. This standalone machine will outperform a cluster node in the majority of cases, for the purpose of running *Virtual Reactor*.

2.3. Plan the Client-Server Configuration

It is possible to configure RLM in several ways, depending on your needs and preferences for using *Virtual Reactor*. If you only have a single machine that will be running *Virtual Reactor* simulations, it may be most convenient to install the RLM server directly on that machine, so that it acts as both RLM server and RLM client:



Fig. 2.1 Single machine acting as RLM server and client

It is also possible for such a machine to act as the RLM server for additional client machines. In the example shown below, two additional large calculation machines are clients, and one laptop is also a client. In general, laptops are not powerful enough to be useful for running large simulations, but it is often convenient to set up simulations on a laptop and then transfer them to a larger calculation machine.

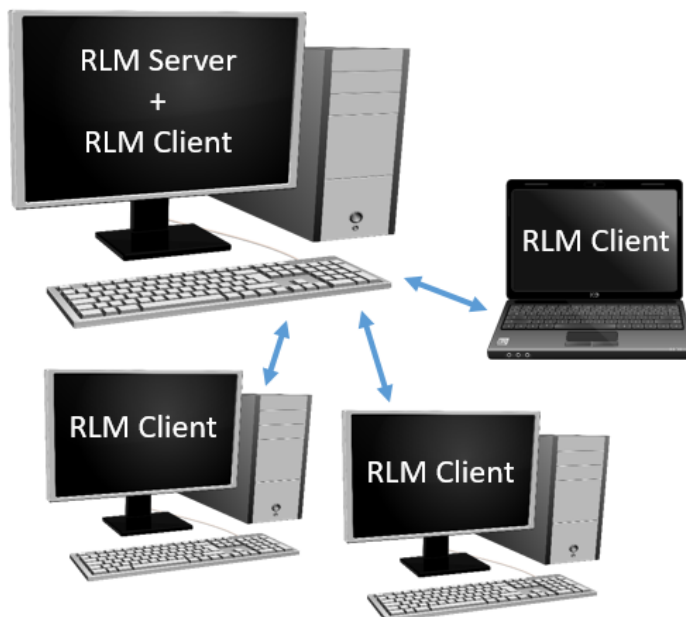


Fig. 2.2 Single machine acting as RLM server and client, with multiple clients

Another option is to have a standalone RLM license server which is not intended to run simulations. This is common when a centralized license server already exists, or when an always-on file server is able to act as the RLM server as well.

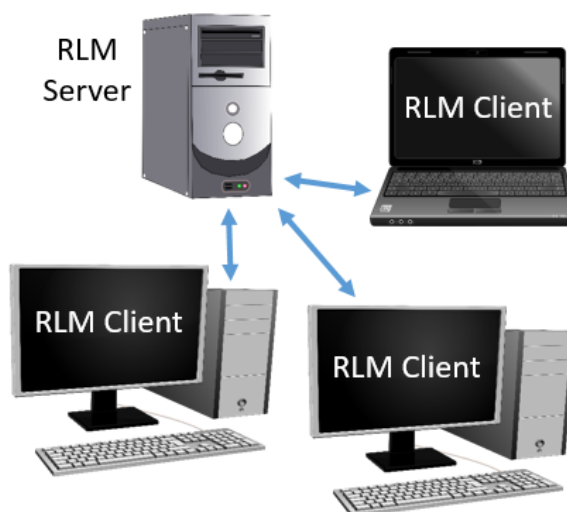


Fig. 2.3 RLM server with multiple clients

For any of these configurations, it is important to note that the RLM server machine must remain on and accessible to the RLM client machines during simulations. If the RLM server is powered off, or loses network connectivity to a client machine that is running a simulation, the *Virtual Reactor* solver will pause and wait for its license to become available again.

Note

The RLM server and all RLM client machines must be on the same network, or the network must be configured to allow all machines to see each other, in order for the *Virtual Reactor* licenses to work.

2.4. Download *Virtual Reactor*

All versions of *Virtual Reactor* are available for download on the CPFD support site:

<https://cpfd-software.com/customer-support/knowledge-base/category/release-versions>

When downloading be sure to choose the appropriate distribution which applies to your operating system (Linux or Windows).

Physical installation media can be sent upon request via email to licensing@cpfd-software.com (please specify Windows or Linux and USB stick or CD).

Once downloaded, the installation files must be extracted from the compressed file by either right-clicking the file with the mouse or using a decompression utility. This will generate the *Virtual Reactor* installation folder in the same directory as the compressed file. You may now [Install the RLM Server](#) (if necessary), or [Install Virtual Reactor](#).

2.5. Install the RLM Server

Note

Administrator (on Windows) or root (on Linux) privileges are required in order to perform the RLM server installation.

Note

You do not need to install or update the RLM server for each new version of *Virtual Reactor*; once the RLM server is set up the first time, it will work with all versions of *Virtual Reactor*.

- If your system will be a single machine acting as RLM server and client with or without multiple clients (it will look like [Fig. 2.1](#) or [Fig. 2.2](#)), you can [Install Virtual Reactor](#), and on the final page, it will give you the option to install the RLM server.

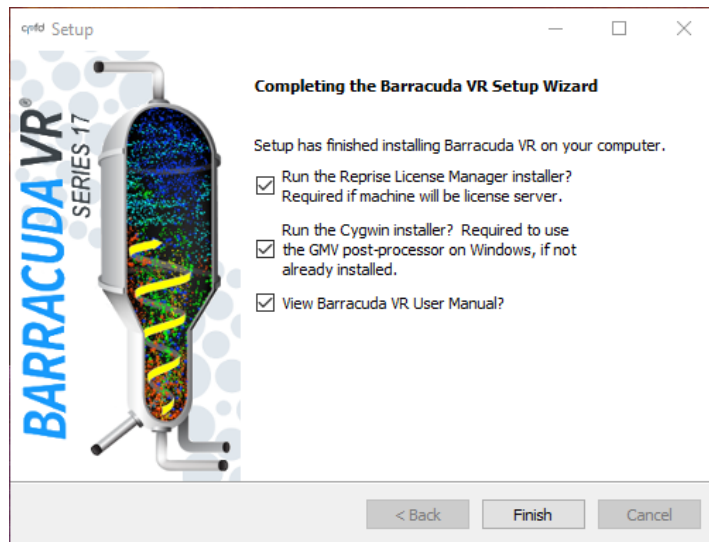


Fig. 2.4 Installing RLM server at end of *Virtual Reactor* installation

- If your system will look like [Fig. 2.3](#), there is no need to run the full *Virtual Reactor* installation. You can install the Reprise License Manager directly by running **reprise-installer** directly from the **reprise** sub-folder of the *Virtual Reactor* installation directory which was [extracted](#).

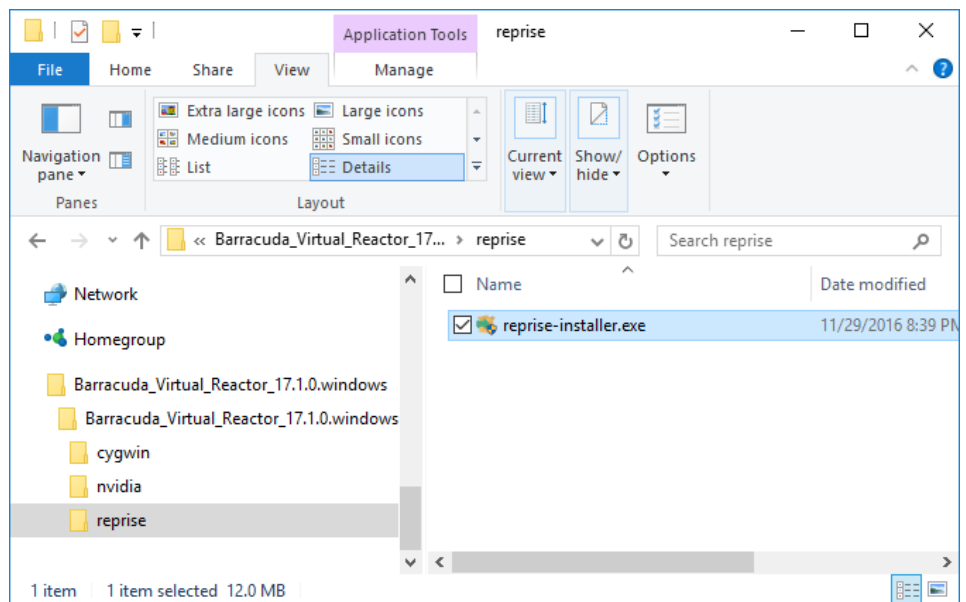


Fig. 2.5 Installing RLM server directly

In either case, at the end of the Reprise License Manager installation, be sure to leave the box checked for *Show system information*.

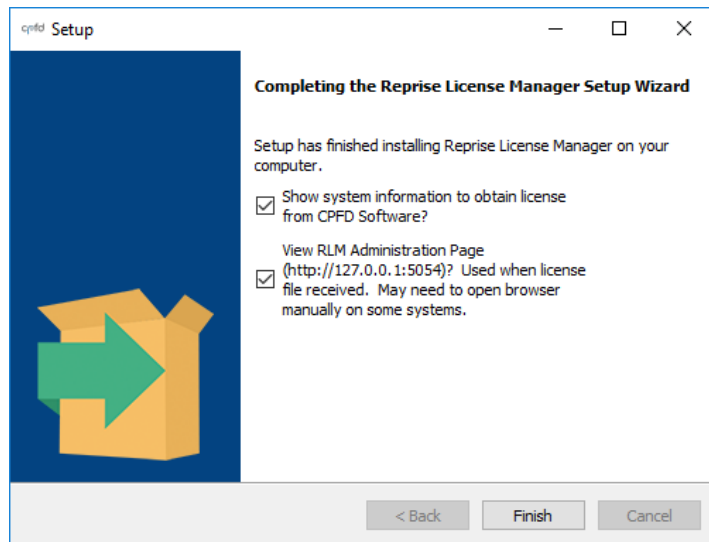


Fig. 2.6 Final screen of RLM installer

A text dialog will pop up showing your system information.

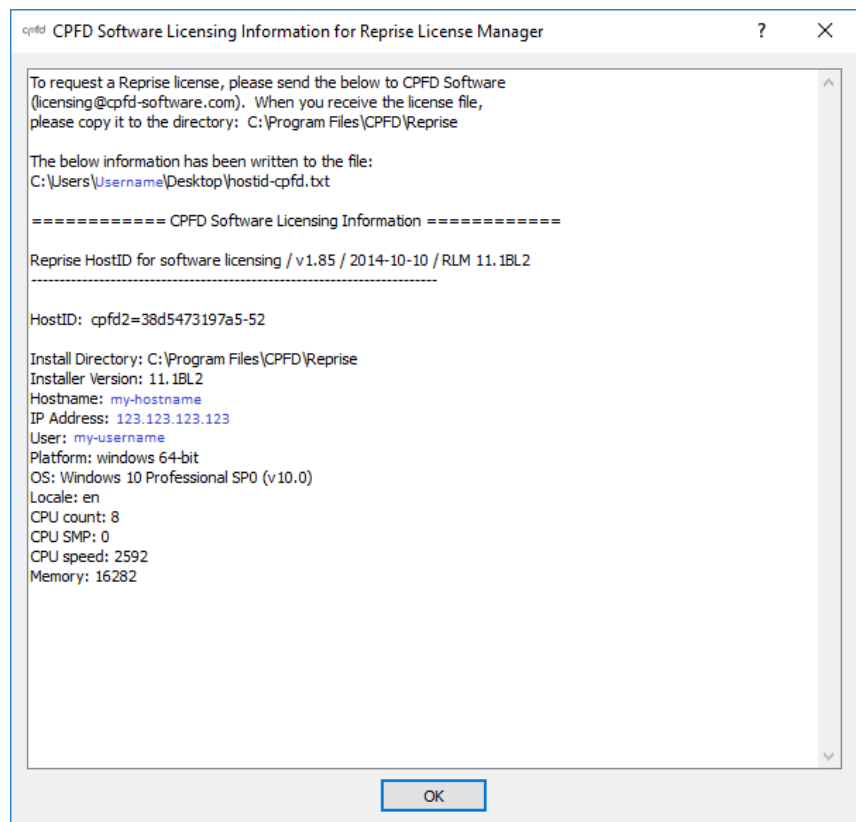


Fig. 2.7 RLM installer host information

Additionally, a text file containing the same information will be saved to your Desktop with a file name of `hostid-cpfd.txt`. Email this file to licensing@cpfd-software.com, and CPFD Software will generate a license file and email it to you.

Note

An alternative method of finding the license server's `hostid` is to run the command `getcpfdid` in a terminal or command prompt.

On Linux, the default installation location of this command is:

```
/usr/local/bin/reprise/getcpfdid
```

On Windows, the default installation location of this command is:

```
C:\Program Files\CPFD\Reprise\getcpfdid.exe
```

2.5.1. Firewall Configuration

In order for RLM client machines to communicate with the RLM server, the server's firewall must have ports 5054, 27015, and 27016 open.

- If the OS of the RLM server is **CentOS 7 Linux**, the firewall ports can be opened by typing the following commands in a terminal as root:

```
firewall-cmd --permanent --zone=public --add-port=5054/tcp
```

```
firewall-cmd --permanent --zone=public --add-port=27015/tcp
```

```
firewall-cmd --permanent --zone=public --add-port=27016/tcp
```

```
firewall-cmd --reload
```

- If the OS of the RLM server is **Windows**, the firewall ports can be opened by using an [Administrator Command Prompt](#). In the prompt, type the following commands:

```
netsh advfirewall firewall add rule name="RLM Web Server" dir=in action=allow  
protocol=TCP localport=5054
```

```
netsh advfirewall firewall add rule name="RLM License Server" dir=in action=allow  
protocol=TCP localport=27015
```

```
netsh advfirewall firewall add rule name="RLM ISV Server" dir=in action=allow  
protocol=TCP localport=27016
```

2.6. Install the RLM License

Once you have requested and received your RLM license file from CPFD Software, it is necessary to install it on the RLM server.

Note

The license file only needs to be installed on the RLM server. It does not need to be installed on client machines.

To install the RLM license file, follow these steps:

1. Save the RLM license file to your Desktop.
2. Copy the license file to the following location depending on the OS of your license server:

Linux

```
/usr/local/bin/reprise/
```

You will need root permission to do this. In a terminal opened to the same directory as the license file, type:

```
su  
<Enter root password>  
cp <license file> /usr/local/bin/reprise/
```

where <license file> is the RLM license file name.

Windows

```
C:\Program Files\CPFD\Reprise
```

Note that Windows Explorer will ask for administrator permission to copy a file into any directory inside C:\Program Files.

3. Open a web browser to: <http://127.0.0.1:5054>
4. Click *Reread/Restart Servers*, then *REREAD/RESTART*:

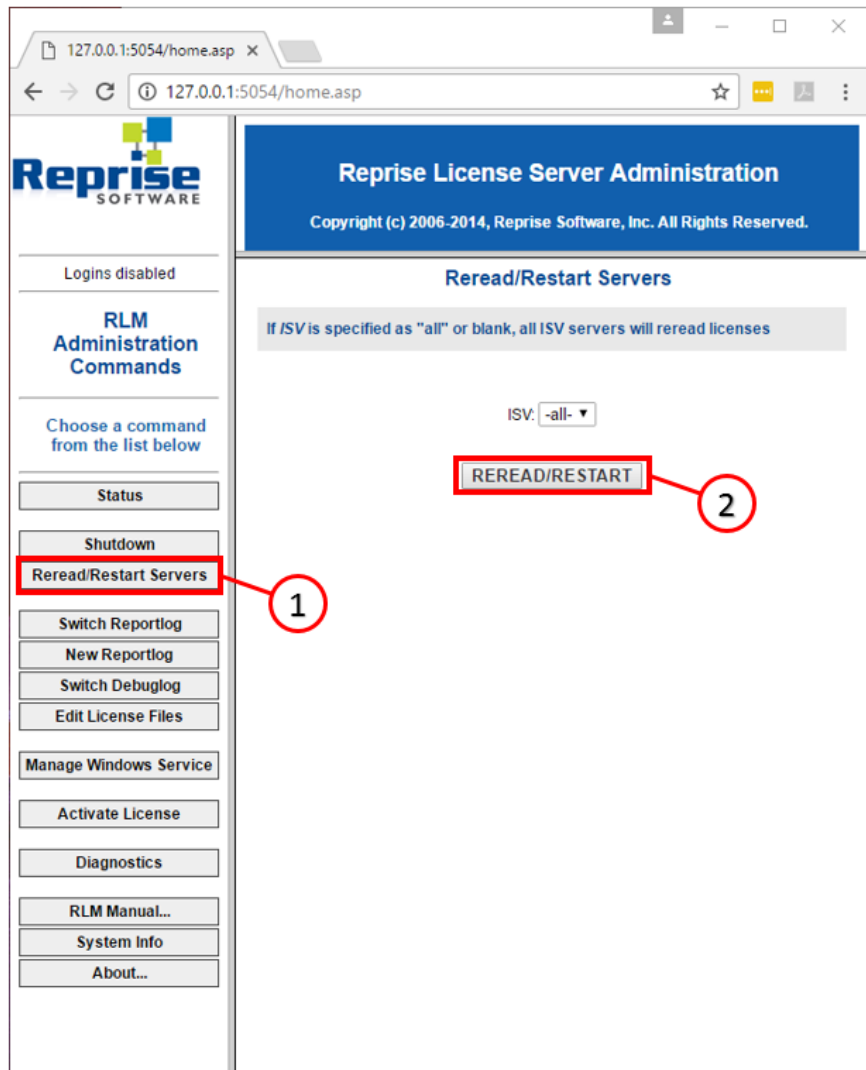


Fig. 2.8 RLM Reread/Restart Servers

Note

It is also possible to request that the RLM server reread its license file(s) via the command-line, in case you do not have access to the web interface of the RLM server. In the `reprise` folder, running the script named `rlmreread` will trigger a reread of the license file(s) for the RLM server. You must have administrator privileges to run this script.

5. Click *Status*, and then click the first *cpfd* button under the *Server Status* column. This lists the current status of your Reprise server licenses and shows licenses available.

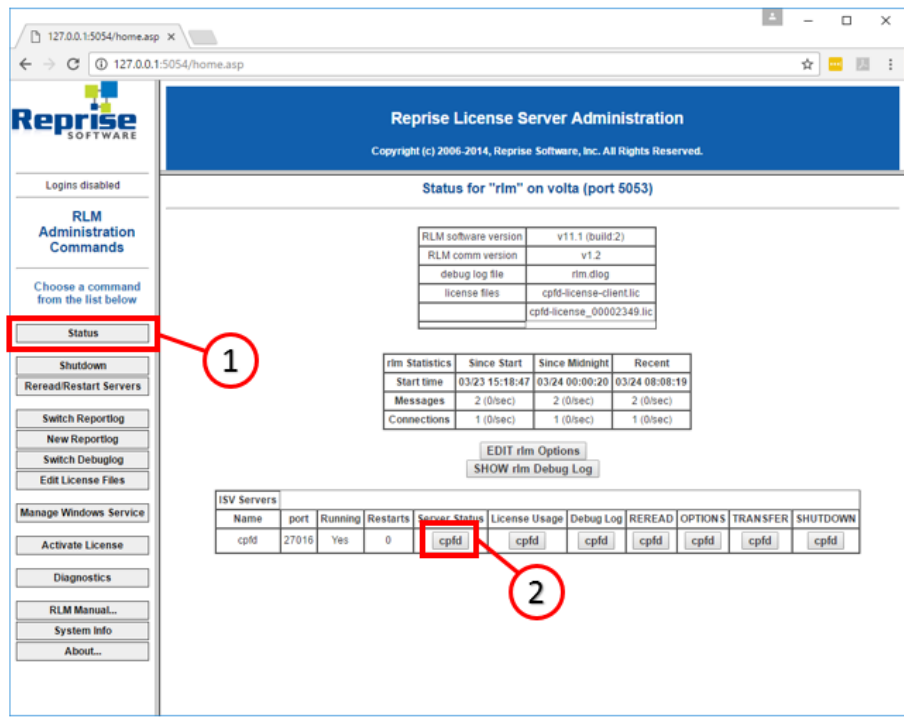


Fig. 2.9 Checking RLM license status

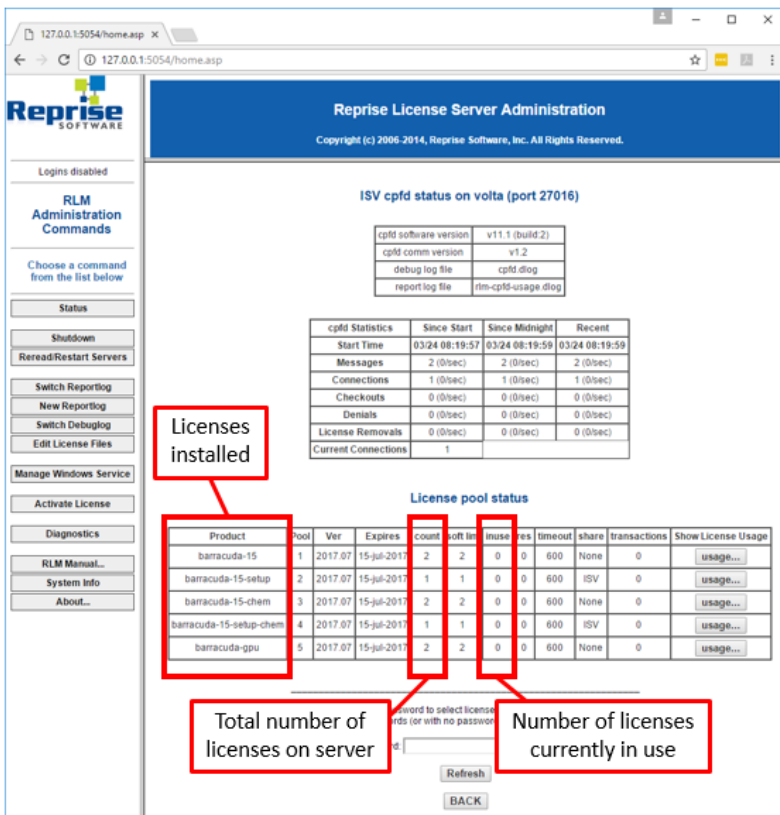


Fig. 2.10 RLM license status table

2.7. Install Virtual Reactor

Virtual Reactor must be installed on every client machine. Multiple versions of *Virtual Reactor* can be installed on a single machine, and each version operates independently. It is not necessary to uninstall old versions of *Virtual Reactor* when installing a new version. [Download Virtual Reactor](#) and then follow the steps below to install the software:

1. Navigate to the *Virtual Reactor* installation folder that was [extracted](#).

2. Double-click on barracuda_setup.run (on **Linux**) or barracuda_setup.exe (on **Windows**) to start the *Virtual Reactor* Setup Wizard. Click *Next*.

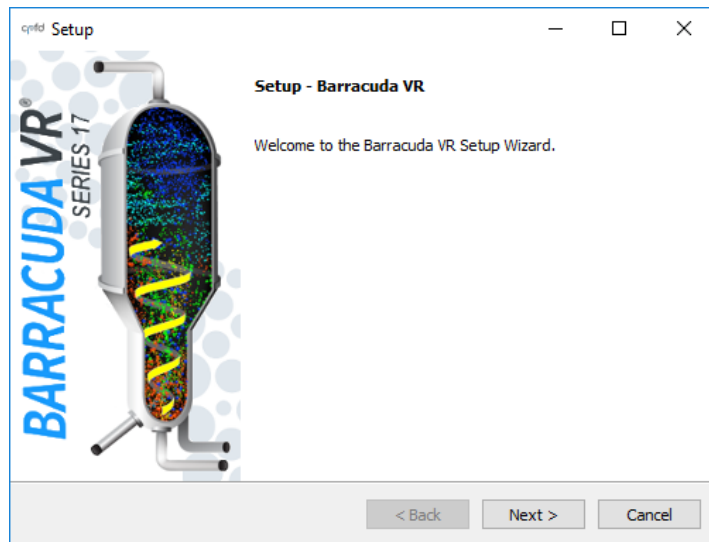


Fig. 2.11 *Virtual Reactor* Setup Wizard

3. Read and accept the License Agreement and click *Next*.

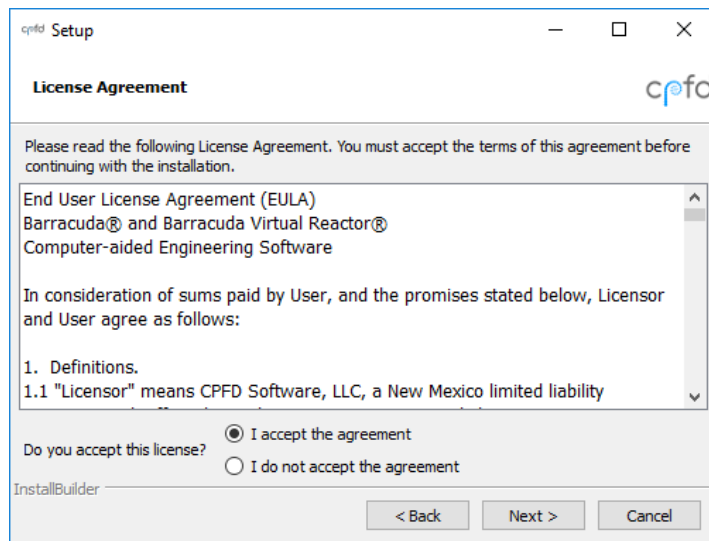


Fig. 2.12 *Virtual Reactor* License Agreement

4. This window shows the default directory in which the *Virtual Reactor* version will be installed. It is recommended to use the default directory. Click *Next*.

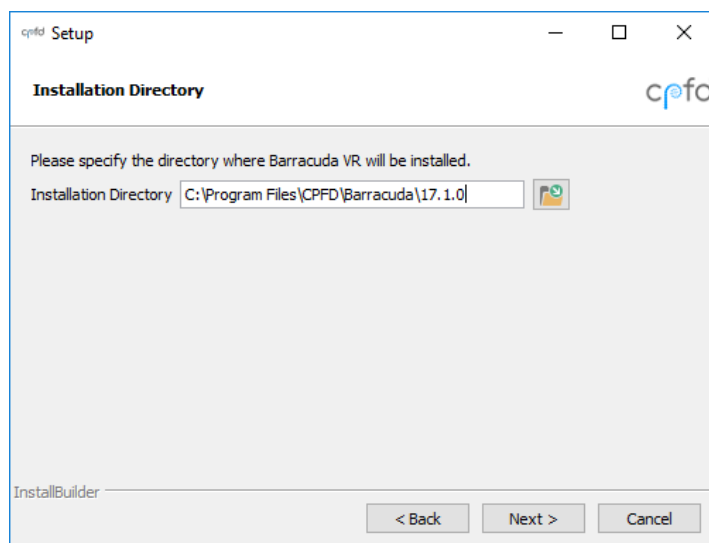


Fig. 2.13 *Virtual Reactor* Installation Directory

5. This window allows you to choose the components to be installed. It is recommended that you leave all components checked and click *Next*.

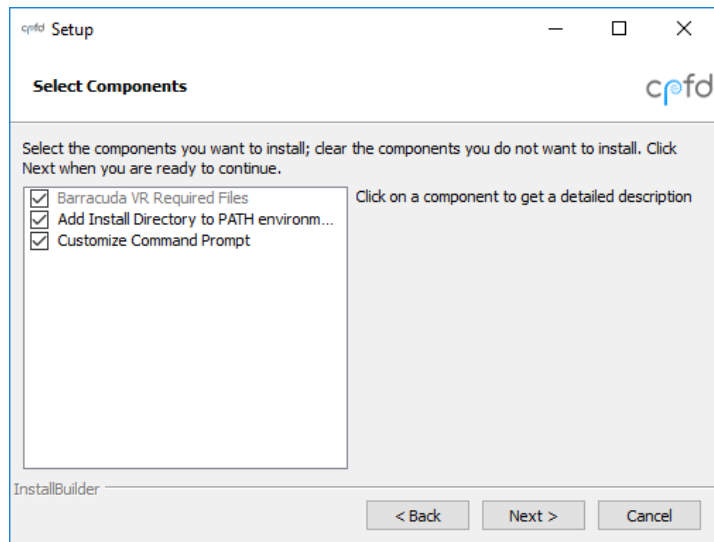
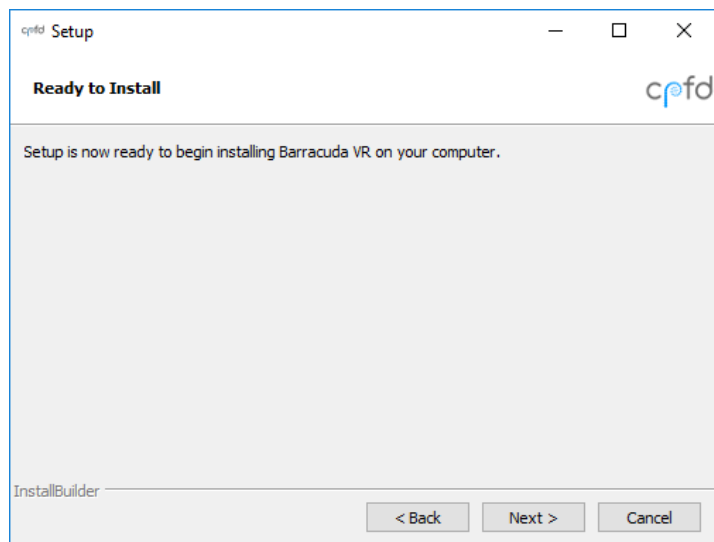


Fig. 2.14 Virtual Reactor Setup Select Components

6. Click *Next* in order to begin the installation.



The installer will display a progress bar as it installs *Virtual Reactor*.

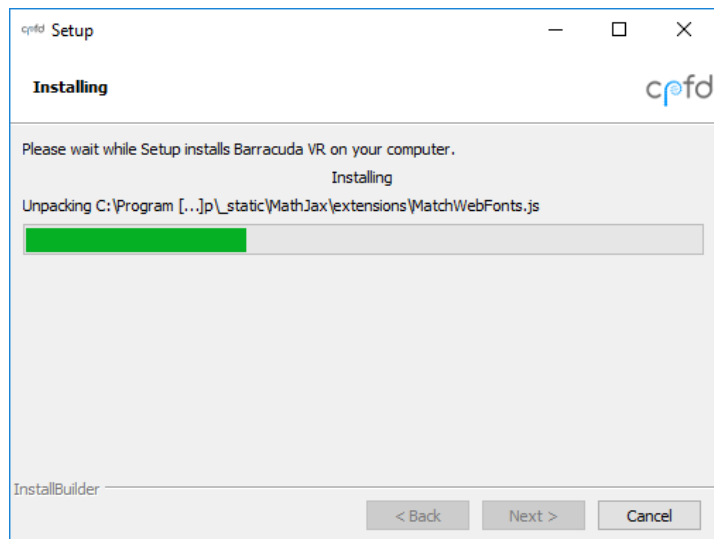


Fig. 2.16 Virtual Reactor Setup Installing

7. Once the installation is complete, the final window of the *Virtual Reactor* Setup Wizard will be displayed. This window shows three options that can be chosen as you finish up the installation process.

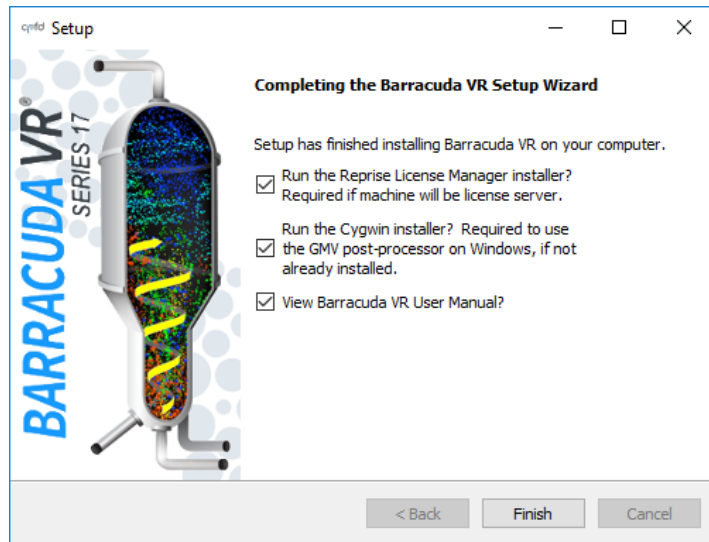


Fig. 2.17 Virtual Reactor Setup Final Page

- *Run the Reprise License Manager installer?* If this is an RLM server machine, leave this box checked. Un-check this box when installing on a client machine. Note: you do not need to install or update the RLM server for each new version of *Virtual Reactor*; once the RLM server is set up the first time, it will work with all versions of *Virtual Reactor*.
- *Run the Cygwin installer?* If this is the first time that *Virtual Reactor* is being installed on a client machine, leave this box checked. After Cygwin has been installed on a client machine, un-check this box for subsequent installations.
- *View Barracuda VR User Manual?* If this is checked, the User Manual will be opened using your default web browser.

2.8. Point Client Machines to the RLM Server

Every RLM client machine must point to the RLM server in order to access the *Virtual Reactor* license(s). The setup for pointing clients to the server must be performed:

- The first time you set up the RLM server and its clients
- Any time the RLM server changes its IP address or hostname; in this case, all client machines need to be updated to point to the new IP address or hostname
- When a new client machine is being configured

Client machines are configured to point to the license server in order to use a license by defining an environment variable called `cpfd_LICENSE`. The first step is identifying the IP address or `<hostname>` of the RLM server. You can use either the IP address or `<hostname>` as the identifier for the RLM server.

- If the OS of the RLM server is **Linux**, you can find its IP address by opening a terminal on the server and typing:

```
ifconfig
```

The IP address is listed as `inet addr` in the printed output.

If you want to use the `<hostname>` of the RLM server, you can find it by opening a terminal on the server and typing:

```
hostname
```

This will print the `<hostname>` of the server machine.

- If the OS of the RLM server is **Windows**, you can find its IP address by opening a [command prompt](#) on the server and typing:

```
ipconfig
```

The IP address is listed as IPv4 Address in the printed output.

If you want to use the <hostname> of the RLM server, you can find it by opening a terminal on the server and typing:

```
hostname
```

This will print the <hostname> of the server machine.

Using the IP address or <hostname> of the RLM server, the `cpfd_LICENSE` environment variable can be defined for the client machine(s).

- If the OS of the RLM client is **Linux**, you can define the environment variable based on the RLM server's <IP address or hostname> by opening a terminal on the client and typing:

```
echo "export cpfd_LICENSE=27015@<IP address or hostname>">> ~/.bashrc
```

Logout and login in order for settings to update.

- If the OS of the RLM client is **Windows**, you can define the environment variable based on the RLM server's <IP address or hostname> by opening a [command prompt](#) on the client and typing:

```
setx cpfd_LICENSE 27015@<IP address or hostname>
```

2.9. Install NVIDIA Drivers

If you will be running *Virtual Reactor* in GPU parallel mode, you must install the NVIDIA drivers for your graphics cards.

- If your calculation machine's OS is **CentOS 6 Linux**, the NVIDIA drivers can be installed by running the following commands in a terminal as the root user:

```
rpm --import http://elrepo.org/RPM-GPG-KEY-elrepo.org
```

```
rpm -Uvh http://www.elrepo.org/elrepo-release-6-6.el6.elrepo.noarch.rpm
```

```
yum install kmod-nvidia nvidia-x11-drv
```

Once installation of the NVIDIA drivers is complete, reboot the system so that they are loaded by the Linux kernel.

- If your calculation machine's OS is **CentOS 7 Linux**, the NVIDIA drivers can be installed by running the following commands in a terminal as the root user:

```
rpm --import http://elrepo.org/RPM-GPG-KEY-elrepo.org
```

```
rpm -Uvh http://www.elrepo.org/elrepo-release-7.0-2.el7.elrepo.noarch.rpm
```

```
yum install kmod-nvidia nvidia-x11-drv
```

Once installation of the NVIDIA drivers is complete, reboot the system so that they are loaded by the Linux kernel.

- If your calculation machine's OS is **Windows**, the NVIDIA drivers can be installed by following the instructions on NVIDIA's webpage for driver downloads:

<http://www.nvidia.com/Download/index.aspx>

2.10. Troubleshooting

We hope you never need to read this section, but in case things aren't working as expected after following the steps outlined above, please review the following troubleshooting tips.

2.10.1. License not found

If the *Virtual Reactor* GUI is unable to find a license file, it will not open. Instead, an error dialog box such as the one shown below will open:

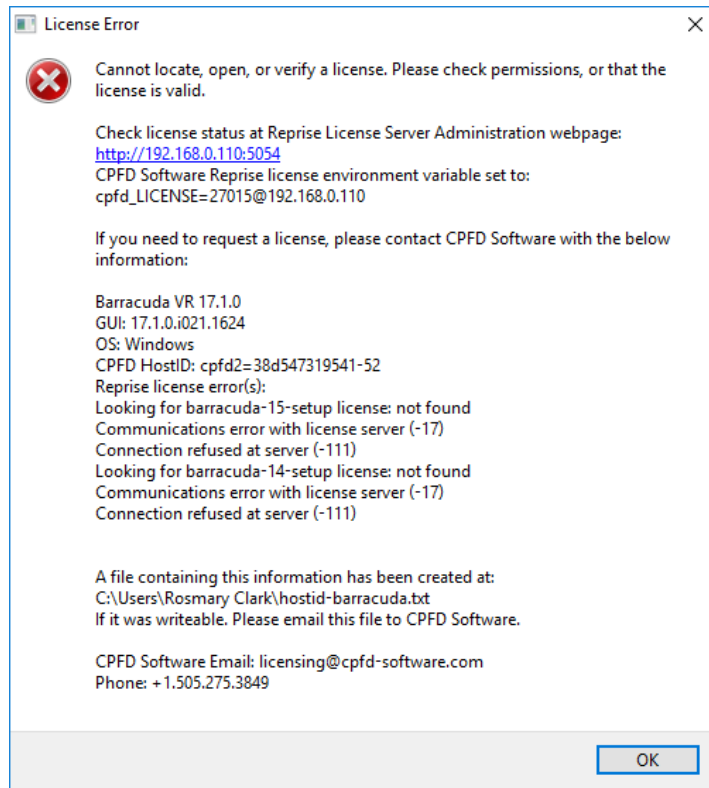


Fig. 2.18 Error dialog shown when the *Virtual Reactor* GUI cannot find a license

If this dialog appears, check the following things:

1. Is the license expired? The license file (.lic) [emailed](#) to you will have the license expiration date as will the RLM license status table (see [Fig. 2.10](#)).
2. Is the IP address or host name of the RLM server correct? [Here's how to check.](#)
3. Is the port number of the license server correct? The default port is 27015, so double-check that the cpfd_LICENSE environment variable is using that port. [Here's how to check:](#)

On **Linux**, type in a terminal:

```
echo $cpfd_LICENSE
```

On **Windows**, type in a CMD command prompt:

```
echo %cpfd_LICENSE%
```

If the port number is not correct, go through the steps in [Point Client Machines to the RLM Server](#).

4. Can the RLM web-page be opened successfully using the hyperlink in the error dialog? If not, then the RLM server is either not running on the server machine, or the client machine is not able to communicate with the RLM server. How to check:

- Ensure that the RLM server is [installed](#).
- Can the client machine **ping** the RLM server? If not, then the client machine is not able to communicate with the server machine. The client and server machines must be able to communicate in order for RLM licenses to be used.

Note

The ping service is not allowed to pass through the Windows firewall by default. It is necessary to [enable ping responses](#) in order to test communication to a Windows RLM server machine.

In order to **ping** a machine, open a terminal (on Linux) or a CMD command prompt (on Windows) and enter the command:

```
ping <hostname or IP address of RLM server>
```

5. Is there a firewall running on the server machine, preventing the client machine from obtaining an RLM license? See [Firewall Configuration](#) for details on how to open the necessary ports for the RLM

server.

6. Is the computer's date and time set correctly? The license manager will not function properly if the date and time is not correct.

2.10.2. NVIDIA Driver Issues

1. After the installation of a new GPU card, some Linux systems may have trouble booting up because the kernel refuses to load the driver module. This can happen because of the secure boot option in the system BIOS. To fix this, either disable secure boot, or add the new GPU card's information to the system's UEFI database.

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