

Schrödinger Product Installation on Linux

The instructions below are for a new installation of Schrödinger software on a typical Linux platform. If you need more details or encounter problems, refer to the [Installation Guide](#), which is included at the top level of the DVD or the download along with these instructions.

Checking your system

1. Check that your system has sufficient disk space:

```
df -h
```

To install all products, excluding Prime third-party software, at least 2.5 GB is needed. 7 GB is required for the PDB, and 4.5 GB for other Prime third-party software.

2. Check that your system version is adequate:

```
uname -r
```

For recent Linux distributions, the version reported should be at least 2.6.9, and preferably at least 2.6.12.

Installing the software

3. If installing from DVD, mount the product DVD.

DVDs are only readable by a DVD-ROM drive or a DVD-R Read/Write or DVD+/-R Read/Write drive. DVD+R Read/Write drives cannot read the DVDs we supply.

If installing from a download, extract the tar file:

```
tar -xvf Schrodinger_Internet_Download.tar
```

4. Change to the top-level directory on the DVD or the download:

```
cd topleveldir
```

For a download this directory should be the subdirectory `Schrodinger_Internet_Download` in the directory you extracted the tar file.

5. Run the install script:

```
sh ./INSTALL
```

Using `sh` is sometimes necessary when installing from DVD.

6. Enter the information requested by the `INSTALL` script.

This includes specifying the installation directory (which is created if it does not exist) and the scratch directory. See [Section 3.3](#) of the *Installation Guide* for details.

7. Set the `SCHRODINGER` environment variable to the installation directory:

```
bash:      export SCHRODINGER=installdir
```

```
csh/tcsh: setenv SCHRODINGER=installdir
```

Setting up access to remote hosts

8. Edit the file `$$SCHRODINGER/schrodinger.hosts` and add entries for all hosts or batch queues on which the software will be run. Do not remove the `localhost` entry.

See [Section 6.1](#) and [Section 6.3](#) of the *Installation Guide* for details. The minimum required for a host entry is
name: *hostname*

9. Set up passwordless `ssh` access between all hosts on which the software will be run.

See [Section 6.2](#) of the *Installation Guide* for details.

10. Perform any necessary cluster configuration (see [Section 6.5](#) of the *Installation Guide*).

Setting up licensing

11. Log on to the license server host (if you are not already logged on to it).

12. Run the `machid` script to obtain information for the license:

```
$$SCHRODINGER/machid > machid.out
```

13. Send the output of `machid` to `help@schrodinger.com` to obtain a license.

14. When you receive the license information, which is sent as an attachment, save it as `$$SCHRODINGER/license`. You can overwrite the existing file, which is a placeholder.

15. On the license server host, start the license server, and check that it is running.

```
licadmin SERVERUP  
licadmin STAT
```

See [Chapter 5](#) of the *Installation Guide* for details.

Checking the installation

16. Run the installation checker:

```
$$SCHRODINGER/run installation_check.pl
```

17. Start Maestro to ensure that it is correctly installed.

```
$$SCHRODINGER/maestro &
```

18. Choose **Manuals Index** from the **Help** menu to ensure that the PDF viewer is working correctly from Maestro.

19. Choose **Online Help** from the **Help** menu to ensure that the browser is working correctly from Maestro.