

Schrodinger Software and License

Much of the information about installing the Schrodinger software and dealing with the license is in the installation guide available here for the 2012 Schrodinger suite:

Dropbox: PMC-AT Research/schrodinger_manuals/suite2012/general/install_guide.pdf

Read chapter 6: "Obtaining and Installing Licenses".

Raj has a 25 token-based library for use with almost all of the Schrodinger software except WaterMap and some other specialized programs. The token-based option comes as a pool of tokens that can be applied to run any program within your library of software programs up to the limit of the total number of tokens. The list below contains examples of some of the programs available and the number of tokens each instance requires in brackets. Multiple instances can be run in parallel to speed up jobs up to the limit of the total number of tokens. Be aware that if you surpass the token limit, your jobs may fail with error messages hidden inside some log file of the job.

- [5] Glide: ligand-receptor docking (requires 6 tokens when run with XP Descriptors on)
- [8] Prime: protein structure prediction package
- [5] Phase: ligand-based pharmacophore modeling
- [5] CombiGlide for combinatorial library design
- [5] Core Hopping: ligand- and receptor-based scaffold exploration
- [2] QikProp: ADME properties prediction of drug candidates
- [4] Liaison: binding affinity calculations
- [1] Epik: pKa calculation in biological conditions
- [1] SiteMap: identification and characterization of active sites
- [1] LigPrep: a 2D to 3D conversion program to prepare ligand libraries
- [3] Jaguar (includes pKa): ab initio quantum mechanics application
- [3] MacroModel: classical molecular modeling application
- [3] ConfGen: bioactive conformational searching
- [4] QSite: QM/MM application
- [1] Strike: scientific data analysis program
- [2] Canvas: customizable cheminformatics platform and interface
- [0] Maestro: unified graphical interface

Workflows

- [8] Induced Fit Docking (Prime + Glide)
- [5] QM-Polarized Ligand Docking (Glide + QSite)
- [1] Protein Preparation Wizard (Epik +Impact (Impact is embedded in Glide))
- [8] Virtual Screening (Epik, LigPrep, Glide, MacroModel, QikProp, Prime)

The license server is currently installed on the following machine:

Hostname: slave003.pmcresearch.com

IP: 75.150.132.105

Type of Machine: x86_64 GNU/Linux

Directory of License server software (as of July 2013): /home/eknoll/SCHRODINGER_64

Current license file: /home/eknoll/SCHRODINGER_64/license

License Dates

The current license file expires August 18, 2013. Raj purchased a year license on December 21, 2012. We had been getting incremental 2 month license files that were renewed every 2 months because Raj had been transitioning to a new cluster. Thus, on Aug. 18 2013, you can get a new license for 2 months or until December 21, 2013. After December 21, 2013, Raj will have to pay for another license.

New 2013 version of Schrodinger Suite

Currently Schrodinger Suite 2012 is installed. This version has worked fine. There is a new version of the `install_guide.pdf` for the 2013 Schrodinger suite if you choose to install this newer version. New instruction manuals come with the software download from Schrodinger. When you upgrade to the new release of Schrodinger Suite 2013, you'll need a new license file (your license for Suite 2012 won't work with the new release). This is unique to this release, and should be the only time this is required. You can download the new version and request your new license file here: <http://www.schrodinger.com/downloadcenter/>

How to get a new license file from Schrodinger:

1. Contact your Schrodinger representative (currently Carrie Weston carrie.weston@schrodinger.com). She will probably email you a week before the current license expires (around August 12, 2013) to remind you to renew the license.
2. Download the latest Schrödinger software, visit the Download Center (login required; Raj has one): <http://www.schrodinger.com/downloadcenter/>
Only do this if you want to install the newest version of the software. The current version has been fine so far.
3. The Schrodinger representative should email Raj a link to a webpage with a form to fill out. Filling out this form will automatically generate a new license file. This file will be emailed to Raj as well as downloadable on the web immediately after filling out the form. This license file must be copied to the license server directory (currently 75.150.132.105: /home/eknoll/SCHRODINGER_64/license) and the license server restarted with the new license file (more instructions below). The form requires you to input information about the machine on which the license server runs (see below).

How to get machine information for the license server:

1. Log onto machine that license server is on. And go to directory that Schrodinger software is installed in.

Currently 75.150.132.105: \$\$SCHRODINGER

You must have the environmental variable setup on the license server machine for your login:

```
export $SCHRODINGER=/home/eknoll/SCHRODINGER_64/
```

This is the schrodinger installation on license server. You may choose to change this directory and the \$\$SCHRODINGER variable with a new installation.

2. Run the command 'machid' from the Schrodinger installation on the license server computer. Currently that would be:

```
75.150.132.105:$SCHRODINGER/machid
```

3. The critical output from the machid command is this:

- a. Host ID: 78e7d1f92ed2 (this is the MAC address of the network card for the current machine)
- b. Machine name: slave003 (this info is requested by Schrodinger, but I don't think it matters. Only the MAC address is important, as the MAC address ties the license server to the physical hardware).

4. This information can be entered into the web form from Schrodinger to automatically generate a license file. The link to the webform is emailed by the Schrodinger representative.

How to restart the license server:

With a new license file, or if the license server is having problems and needs to be rebooted:

\$\$SCHRODINGER == schrodinger installation on license server, which currently is /home/eknoll/SCHRODINGER_64/

1. Stop the current license server, if it is running:

```
$$SCHRODINGER/licadmin STOP
```

2. Replace the old license file with the new one:

```
mv $$SCHRODINGER/license $$SCHRODINGER/license.old.date
```

```
cp <newLicenseFile> $$SCHRODINGER/license
```

3. Restart the license server daemon:

```
$$SCHRODINGER/licadmin START
```

4. To check the status of the license:

```
$$SCHRODINGER/licadmin STAT
```

If have problems with License Server

If you encounter any errors please use the 2012 Diagnostics Tool. To run the diagnostics tool please enter \$\$SCHRODINGER/diagnostics in a terminal window. Note, you may not be able to run this diagnostics tool from the remote license server because this server may not be setup to forward GUI windows. If there are problems, contact Eric or Schrodinger. Alternatively, you can do the following:

If the license server is on a remote machine and you are encountering errors, you should run the following five steps on both the license server and on your local machine:

1. Open a terminal window.
2. Set the SCHRODINGER environment variable to point to your software installation.
3. Enter the command `$SCHRODINGER/licadmin INFO`.

When the licadmin program finishes, it prints a message telling you the name of the file it created. The name is in the form `username-machine-license-info.tar.gz`. This file should be in the current directory.

4. Rename the file to `username-machine-license-info.tarball`. This is necessary because some mail programs filter out files with a `.tar.gz` extension.
5. Send the renamed file to `help@schrodinger.com`.

If you have other questions or problems please see our online knowledge base at: <http://www.schrodinger.com/kb/> and type 2012 Linux in the search box.

How to connect to the remote license server to run Schrodinger software

After the license server is running with the correct license file, as described above, you will want to connect to this license server to get permission to run the Schrodinger software. The method described here is one way to do it. There are other ways described in the `install_guide.pdf`.

The Schrodinger software can be installed on any Linux, Mac or Windows machine. The installation does not require a license. It only requires access to the installation files, which can be downloaded from Schrodinger with the proper login credentials (Raj has this). Thus, the software is installed without the license, but it will not run. It can only run with a license, either locally (as a local license file – not the type Raj currently has) or the software on a remote machine must contact the license server running on the license server machine to check out tokens (this is the type of license Raj currently has).

These instructions are for creating an SSH tunnel on a linux or mac osx system. This SSH tunnel creates a connection between the license server and your machine (or compute nodes) where you are running the software. Be aware that there are other ways to do this, especially if you are running a cluster with a proper job queuing manager. The advantage of the method described here is that it will work with any machine anywhere on the Internet that has the Schrodinger software installed and that can ssh to the license server machine. In order to ssh to the license server machine, you need an account and password, which Raj can provide.

For creating the SSH tunnel on a Windows machine (if you installed the Schrodinger software on a Windows machine), you can use Putty, but the steps will be slightly different. I would google "putty ssh tunnel" to find instructions on how to do the SSH tunnel with putty.

From a terminal on host (i.e, the client, as in your laptop or workstation on which you run Maestro or other Schrodinger software)

1. Open terminal;
 - o keep this terminal open so that ssh port tunneling remains running
2. Create SSH tunnel to license server at PMC.
 - o `ssh -f -N -g -L 27008:75.150.132.105:27008 -L 53000:75.150.132.105:53000 <yourUserName>@75.150.132.105`
 1. note: this forwards 2 ports: 27008 and 53000
 2. -f fork and run the ssh port forwarding in background
 3. -N do not execute a command. Needed when -f running in background, otherwise expecting a command rather than just tunneling
 4. -g Allows remote hosts to connect to local forwarded ports.
 5. -L port forwarding (tunneling)
3. Set up environmental variables on linux, if not already in ~/.bashrc on client (your machine)
 - o `export SCHROD_LICENSE_FILE=27008@localhost`
tells schrodinger software to look at port 27008 on local host
 - o `export SCHRODINGER=/opt/schrodinger/suite2012/`
you should fix this to point to the directory you installed software on your computer
4. Start Maestro
 - o `$$SCHRODINGER/maestro` # add '-SGL' option for Linux VM. On Mac OS X can omit
 - o Need to start maestro from same terminal that setup ssh tunnel and environmental variables, rather than through Mac Finder or other GUI clicking.

Diagnosing problems with the SSH Tunnel

The following is a list of common problems you could encounter with the SSH tunnel method.

1. License server is not running on the remote license server machine. Or the license has expired. How to check:
Make sure Schrodinger FlexLM license server is running at 75.150.132.105
 - o `ssh <yourUserName>@75.150.132.105`
 - o `cd $$SCHRODINGER` # schrodinger installation dir on license server
 - o `./licadmin STAT` # status of license server with list of 25 tokens for schrodinger software
 - o # If need to restart server because above command does not show tokens for software:
 - o `./licadmin STOP`
 - o `./licadmin START`

2. You don't have a proper login name and account on the server at 75.150.132.105

Ask Raj to get you an account

3. You reset the license server with a license file that has different ports.

- o The first 2 lines of the current license file installed on 75.150.132.105:\$SCHRODINGER/license are:

```
SERVER slave003 78e7d1f92ed2 27008
```

```
VENDOR SCHROD PORT=53000
```

- o Note the '27008' and '53000'. These are the port numbers under which the license server does certain things, and they must match the port forwarding in the SSH tunneling in step 2 above.

4. The SSH tunneling got messed up. You need to kill the previous instance of the ssh tunnel you created. First, find the process ID (PID) number for the ssh tunnel on your client machine (where you're running the Schrodinger software). You can use either of the following commands (at least on OS X): lsof or ps

- o `lsof -i -n -P | grep ssh`

#output:

```
ssh 16041 UserName 3u IPv4 0xffffffff80207f44e0 0t0 TCP 192.168.1.10:49873->75.150.132.105:22 (ESTABLISHED)
```

```
ssh 16041 UserName 5u IPv4 0xffffffff8032236de0 0t0 TCP *:27008 (LISTEN)
```

```
ssh 16041 UserName 6u IPv6 0xffffffff80207f29c0 0t0 TCP *:27008 (LISTEN)
```

```
ssh 16041 UserName 7u IPv4 0xffffffff80323b5160 0t0 TCP *:53000 (LISTEN)
```

```
ssh 16041 UserName 8u IPv6 0xffffffff80207f2600 0t0 TCP *:53000 (LISTEN)
```

- o `ps aux | grep ssh`

#output:

```
UserName 16041 0,0 0,0 2435188 344 ?? Ss 9:06pm 0:00.00 ssh -f -N -g -L 27008:75.150.132.105:27008 -L 53000:75.150.132.105:53000 eknoll@75.150.132.105
```

- o Note the PID in the 2nd column of either of those commands is 16041 in this example. This PID is used to KILL the ssh tunnel. There may be other SSH processes running on your machine, and thus other output from the above commands. The way to distinguish is to look for the port numbers used in the SSH tunnel of 27008 or 53000.

- o If you can't find a PID with those port numbers from the lsof or ps commands, then your SSH tunnel is not running. Go directly to restarting the SSH tunnel.

- o Kill the SSH tunnel:

```
kill -9 16041 #note, your PID will be different than 16041 shown here.
```

- o Restart the SSH tunnel.

```
ssh -f -N -g -L 27008:75.150.132.105:27008 -L 53000:75.150.132.105:53000 <yourUserName>@75.150.132.105
```