Sorcerer Setup Guide

For Sorcerer PE V3.4 and Above

Release V1.2

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Table of Contents

Introduction

This document describes how to set up a new Sorcerer system for searching, and discusses some special configuration tasks that may sometimes be required. For routine operation of Sorcerer, see the Sorcerer User Guide. The material contained herein describes Sorcerer with release 3.4 or above of Sorcerer PE software.

This manual is intended for the person who is in charge of setting up and maintaining the Sorcerer system. For basic use, this does not require specialist IT knowledge, and this document just assumes general familiarity with desktop computing concepts. Some advanced sections may require more IT expertise; these are identified where they occur in the text.

Basic Installation

Preinstallation Considerations

Sorcerer is delicate and is susceptible to damage or dislocation that may not be apparent from the outside if not handled carefully. Some models are also heavy (up to 90lbs). Proper arrangements should be made in shipping, unpacking and moving Sorcerer units to avoid the possibility of damage to the unit, or of injury to personnel. Do not attempt to install or connect a unit that has, or appears to have sustained physical damage.

For the integrity of the system and your own safety, ensure that a properly wired and grounded power outlet is available for Sorcerer, and that the A/C power meets the specifications given below for each Sorcerer model. Do not apply power in the presence of moisture. Internationally, a standard 3-pin computer power cord with a plug appropriate to the local outlet type is required. This replaces the US type power cord shipped with the unit.

A monitor, a USB keyboard and a USB mouse are required for initial setup of the unit, and are useful, but not required, for routine operation. For the monitor, a resolution of 1024×768 or greater is recommended. These devices are not included in the product and should be obtained separately.

For use over a network, an RJ-45 10/100/1000 BaseT ethernet connection is required. By default, Sorcerer is configured as a DHCP client to obtain a network address from a server.

The following network services and ports are required to be routed for Sorcerer clients

- HTTP (port 80/tcp)
- ssh (port 22/tcp)
- smb (optional, but recommended) (ports 137/udp, 138/udp and 139/tcp)

Sage-N Research strongly recommends that where possible, its customers should provide Sage-N Research technical support personnel internet access to Sorcerer in order to make support

as effective as possible. A convenient, secure method for doing this is by using a VPN ("Virtual Private Network") Connection. This can often be set up in institutional networks for this purpose —please consult with your network administrator.

Sorcerer products are supplied in two physical configurations, which are addressed in detail below:

- A deskside tower — the Sorcerer 2 Tower network appliance for workgroups, and its single-user derivative, the Sorcerer Solo
- A rackmount chassis — The Sorcerer 2 Rack system

Sorcerer 2 Tower and Sorcerer Solo Specific Considerations

The Sorcerer deskside tower configuration places minimal demands on its environment:

- Dimensions: 18.35" H × 11.26" W × 29.33" D desktop/deskside space.
- Grounded 3-pin outlet outlet (or international equivalent outside US): 110-240V auto-sensing, 15A@115V, 47-63Hz.
- Typical office temperature and humidity control

Sorcerer 2 Rack Specific Considerations

The Sorcerer 2 (Rack) is designed for deployment in a server room, and for maintenance by IT personnel:

- Dimensions: 3.38" H × 19.0" W × 30.31" D for mounting in industry-standard 19" rack.
- Grounded 3-pin outlet outlet (or international equivalent outside US): 110-240V auto-sensing, 15A@115V, 47-63Hz.
- Typical server room temperature and humidity control

Initial Setup of Sorcerer 2 Tower/Rack and Solo

Follow these steps:

- *(Sorcerer 2 Tower and Sorcerer Solo only.)* Locate a spot for the Sorcerer near a power outlet and a network connection.

Ensure unimpeded air circulation and ascertain that the unit's vents will not be blocked. Normal office ambient conditions (with air conditioning if appropriate) are suitable for Sorcerer.

- *(Sorcerer 2 Rack only.)* Sorcerer 2 Rack is designed for mounting in an industry standard 19" rack. It requires 2U of rack height, and 28.74" of depth.
- Carefully unpack Sorcerer. Do not drop or jar the main unit as it is sensitive to shocks. When lifting unit, use caution and, if necessary, assistance from skilled installers. **The unit is heavy and may cause injury if improper maneuvering is attempted.**
- Check the packing list to ensure all items are present. Retain packing material (including pallet, if used) in case it is ever required for moving or reshipping a unit.
- If you have confirmed that your network meets the requirements as specified under Preinstallation Considerations, then plug Sorcerer into the network using an ethernet cable. If your Sorcerer is furnished with multiple Ethernet ports, use port 0 (typically the one adjacent to the monitor connection), to avoid licensing problems.
- Attach monitor (not included in product) to Sorcerer using the standard VGA connectors.
- Attach a USB keyboard and a USB mouse (not included in product) to USB connectors on the unit.
- Switch off (if possible) the wall outlet to be used. Attach the power adapters and cables for the main system unit and monitor. Plug into a power outlet, taking precautions to avoid exposure to live connectors. Turn wall outlet switch on. In some Sorcerer models, there may be an additional power switch near the power cable connection: if so, switch it off while connecting cables, and then back on afterwards.
- Power the unit up by pressing the power button on the front panel, and wait 2-5 minutes for the Sorcerer login prompt to appear.

Logging in to Sorcerer: Account Names and Passwords

In routine operation, all access to Sorcerer searching is through the `sorcerer` user account. You can use this login either at a

command line shell, either when using Sorcerer remotely at the command line, or when you have reconfigured the system as a standalone workstation. The same user ID and password will be required for access to the SAMBA file server from Windows Explorer. The default password as supplied by Sage-N Research for the `sorcerer` user account is `sagen`.

System maintenance activities such as network configuration may require using the administrator account, which is called `root`. This account has complete permission to do anything on the system, including destroying the entire setup. Only use this account when absolutely necessary and be very careful when you do. Again, standard use of Sorcerer does not need this account, and if you damage the configuration when using it, we at Sage-N Research may not be able to support your changes. For security reasons, the default `root` password is not published here, but we will supply it to a customer on request.

Using Sorcerer as a Network Server

The Sorcerer is primarily designed to be used as a network appliance from client computers, although it may also be used as a stand-alone workstation, when augmented with a monitor, keyboard and mouse to interact with the system.

Sorcerer needs no network configuration if it is set up as a drop-in network appliance using DHCP. This is often the default for local area networks, if your network administrators have not adopted another policy. Specifically, Sorcerer needs no network configuration for networks meeting the following specifications:

- DHCP server on the network (this means that computers plugged in the network automatically get their network address from this server)
- No existing Sorcerer installation on the network
- Computers being used as Sorcerer clients have the following network setup:
    - An ethernet adapter with TCP/IP active
    - Windows clients have netBIOS over TCP/IP enabled (typically it is enabled by default).
- Certain network protocols and ports (http in particular, but also smb for Windows file sharing, and for some advanced

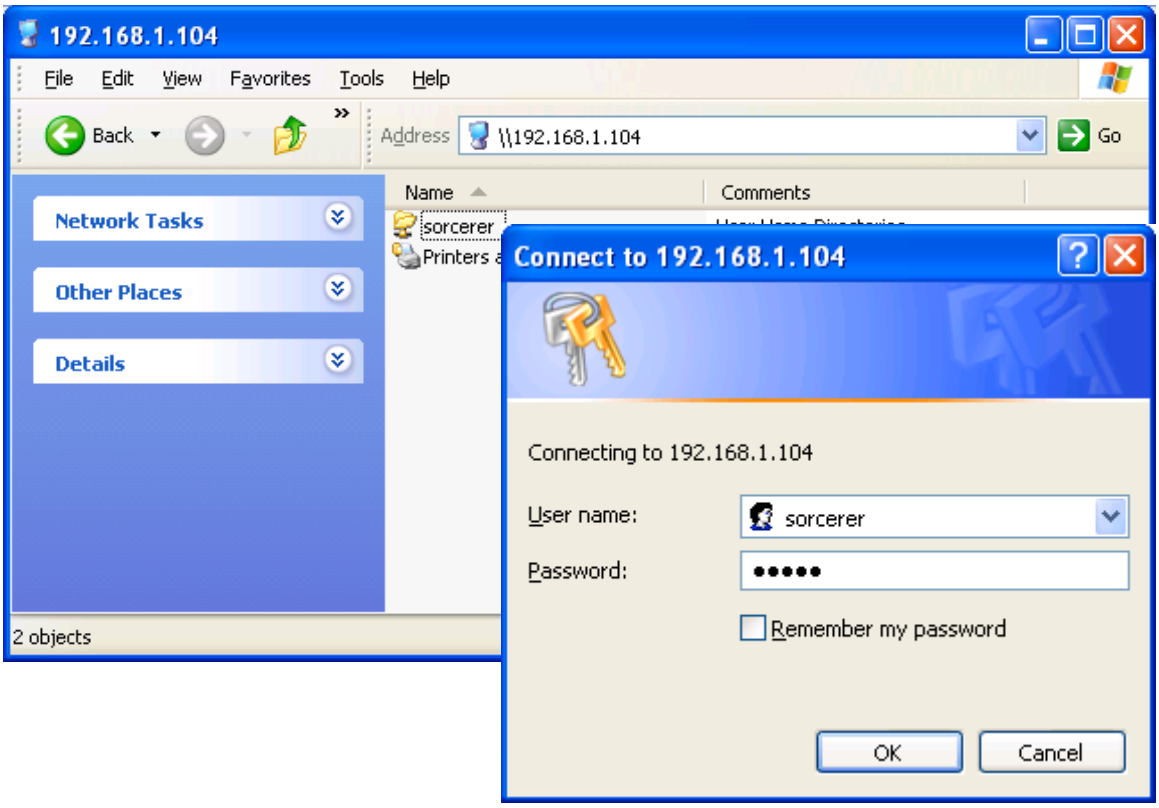
applications, ssh) are fully routed to Sorcerer (they usually are unless there's a strict firewall in between)

For other network configurations, including setting a static IP address, please consult your network administrator as to requirements and refer to Advanced Network Setup, below.

Using Sorcerer in a Windows Environment

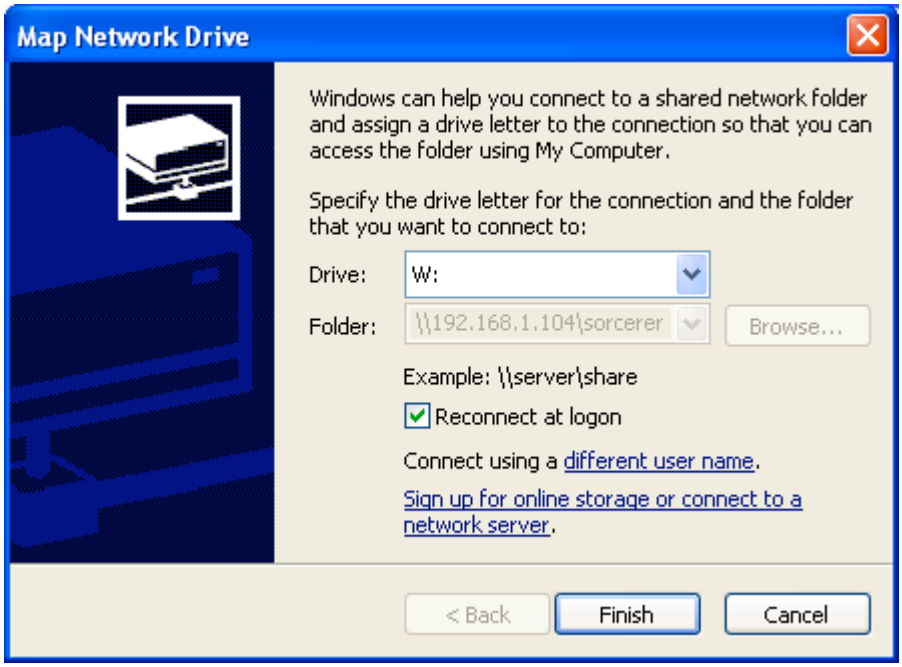
Sorcerer also supports Microsoft Windows File Sharing, which is a convenient way of uploading and downloading files to and from Sorcerer. The service used for this is called SAMBA, which makes files on Linux servers (such as Sorcerer) look as though they are on a Windows File server.

- The default name is `sorcerer-pe` in workgroup `SORCERER` on the Microsoft Windows Network.
- Using Windows Explorer, look for that server name, e.g. `\\sorcerer-pe`. (There's sometimes a delay in Microsoft Windows Networking before a computer shows up in the Entire Network list — either wait a few minutes or search for the computer name explicitly.)
- Alternatively to using the Samba network name, you can just use the IP address of the Sorcerer together with the Windows server notation, e.g. `\\192.168.1.104.`



- You will be prompted to enter a user name and password. Use the standard `sorcerer` user name, for which the default password is `sagen`.
- On Windows computers, you can also use the Samba name for web access to Sorcerer — Enter the URL: `http://sorcerer-pe/`. (Users on other systems will need to use the IP address instead – see Accessing Sorcerer from non-Windows Computers below.)

Once you find the server, it's convenient to map the drive for future use. Right click the `sorcerer` home folder and choose the `Map Network Drive...` option


Map Network Drive
Windows can help you connect to a shared network folder and assign a drive letter to the connection so that you can access the folder using My Computer.
Specify the drive letter for the connection and the folder that you want to connect to:
Drive:
W:
Folder:
\\192.168.1.104\sorcerer
Browse...
Example: \\server\share
Reconnect at logon
Connect using a different user name.
Sign up for online storage or connect to a network server.
< Back
Finish
Cancel

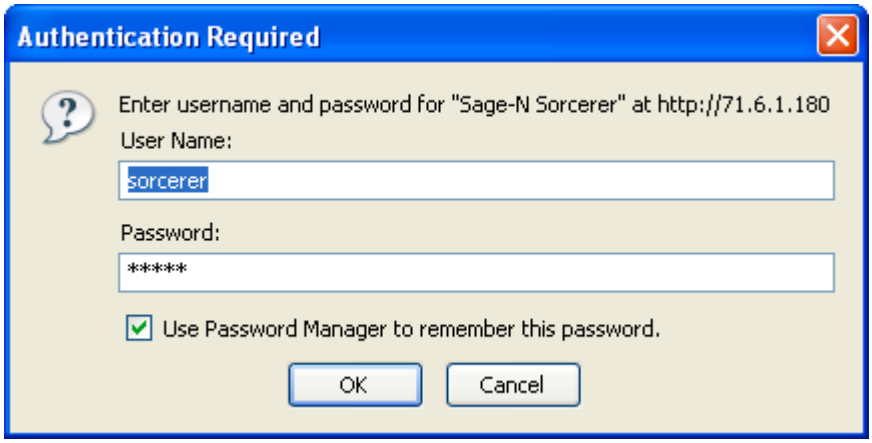
Interacting with Sorcerer

There are three main ways of interacting with Sorcerer for set-up and configuration tasks:

- Using the Sorcerer Web GUI in a web browser, either on Sorcerer itself, or on a networked computer
- Using graphical tools on the Linux desktop in GNOME, the graphical user interface
- Using the Linux command line

Using the Sorcerer Web GUI

The Sorcerer GUI is primarily designed for users on networked computers to do searches, but it also provides some tools for administrators. In this case, you can use the GUI from any networked computer, by typing the network address into a Web browser. Firefox, Internet Explorer 6 or Safari is recommended for best results. At the prompt, enter the user name `sorcerer` and the password, which by default is `sagen`.



The system management tasks which can be performed from the Web GUI include:

- Transfer of data
- Management of protein and peptide databases
- System information (software version numbers)
- Entering a license key

- Setting the Web GUI password
- Displaying the license agreement (EULA)

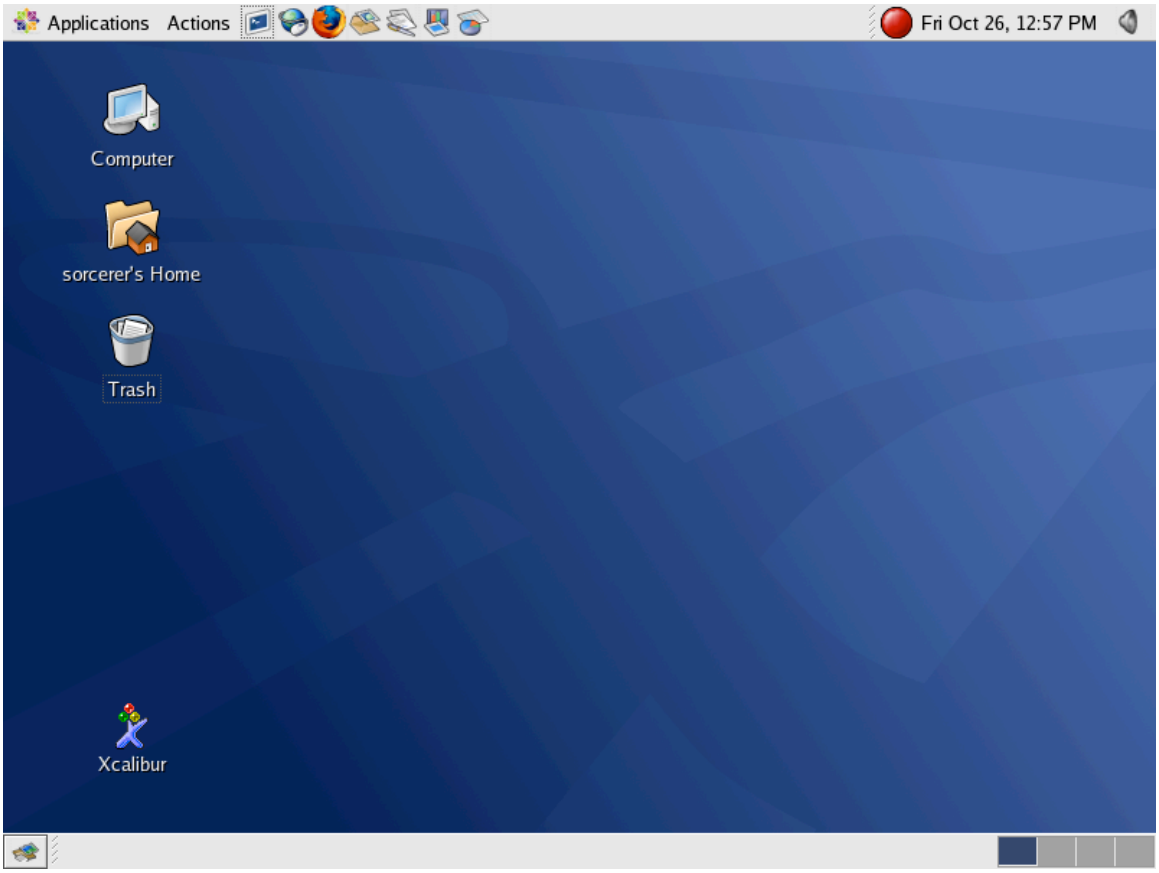
Linux Desktop Tools

Most network configuration tasks can be performed with graphical tools using the menus and icons on the Linux desktop graphical user interface of Sorcerer. This is more convenient and friendly for most people than using Linux commands. However, it is only available when you are sitting in front of Sorcerer with a monitor attached, and not over the network.

The GUI doesn't run by default, so you do have to deal with the command line briefly to start it up. When Sorcerer is ready, it will display a login prompt. Type the user name and password, and then, and the command prompt, type `startx`.

```
CentOS release 5 (Final)
Kernel 2.6.18-el5 on an x86_64
Localhost login: sorcerer
Password:
[sorcerer@localhost ~]$ startx
```

After a few seconds, you will see the Linux desktop appear on the monitor.



This is the Gnome User interface, which operates similarly to other windows-based systems. You can open programs and configure settings from the menus on the top bar, you can click or double-click icons to open files or programs, and you can right-click objects for a context menu applying to each object. Further information is available from the the Help menu.

The Linux Command Line

In basic operation of Sorcerer, you will not need to use the Linux command line. This section is provided for those who may need to do more advanced setup tasks or who are comfortable using Linux.

The Linux command line can be accessed from a monitor and keyboard attached to Sorcerer, in which case you log in as described above. Alternatively, the command line can be used over the network by logging in remotely from another computer. This is especially useful when Sorcerer is set up as a headless server in routine operation.

In order to access Sorcerer across the network, you will need to use the ssh ('secure shell') protocol. Unix (including Mac) and Linux systems typically have these programs built into the OS, but from a Windows machine, the following software is recommended, available from `http://www.chiark.greenend.org.uk/~sgtatham/putty/`:

- PuTTY -- an ssh command line client
- PSCP -- an scp remote copy utility (optional)

PuTTY is a shell that runs on Windows that allows you to run commands on a remote Linux system, in this case, Sorcerer. (PSCP, which you run in a MS-DOS command prompt, can also be useful for copying files to and from Sorcerer as a command line alternative to using SAMBA.)

When PuTTY is run on Windows, you are prompted for a Host Name or IP Address (e.g. sorcerer_pe or 192.168.0.2), a Port (should be 22) and a Protocol (we are using ssh). ssh is very careful about security and verifying connections, and so it may throw up messages asking you confirm the settings. On a trusted, firewalled internal network, you can cheerfully accept these and enter your user name and password. These will be `sorcerer` and `sagen` for normal operation of Sorcerer, but you may use a root account for some more potentially dangerous and therefore protected operations.

Advanced Configuration

Usually, the steps outlined in the section Basic Installation will be fine to set Sorcerer up on most networks. Sometimes, particular local circumstances and policies will require customized configuration. Sorcerer is a Linux-based system with many networking options that can be changed in such an environment by a knowledgeable network administrator.

Please note: any change from default settings is the responsibility of the customer, and Sage-N Research, Inc. will not be responsible for supporting customized configurations. If problems arise with such configurations, support may be limited to restoring default settings, possibly by completely re-installing all software and/or placing the system on a stand-alone network, as described under Stand-Alone Network Configuration.

Advanced Network Setup

Fixed IP Addresses

A common custom requirement is to assign a fixed IP address, instead of a changeable one allocated by DHCP. Such an address can also make it easier to access Sorcerer using that address, as an alternative to using the Samba name. A fixed address can be provided either by configuring it on the DHCP server or by assigning an IP address statically. The former approach is preferable since it does not require a change to Sorcerer's network configuration. Most DHCP servers, including those built into routers, can be set up to recognize where a DHCP request is coming from and assign a predetermined address at that time. However, if that is not possible, then setting the IP address statically is an alternative.

Open the Network Configuration control panel (choose Administration ▸ Network from the System menu in the Linux desktop). You will need to supply the root password. Double-click the entry for the active Ethernet connection (typically eth0). Press the ‘Statically set IP addresses’ radio button and supply the address settings.

Determining the MAC Address

Some network administrators use DHCP to automatically assign internet addresses, but the servers may require the new client computer to be a specific, identifiable system. This is generally done using the MAC address, a unique number that is associated with the Ethernet adapter of the system. You may need to find this number to give to your network administrator before you plug the system in.

To find out the MAC address, type `/sbin/ifconfig` for the active Ethernet connection, usually `eth0`. Note the value in the `HWaddr` field, a number like 00:0D:60:84:55:1E.

```
[sorcerer@71-6-1-180 ~]$ /sbin/ifconfig eth0
eth0      Link encap:Ethernet  HWaddr 00:0D:60:84:55:1E
          inet addr:71.6.1.180  Bcast:71.6.1.191  Mask:255.255.255.240
          inet6 addr: fe80::20d:60ff:fe84:551e/64 Scope:Link
          UP BROADCAST RUNNING MULTICAST  MTU:1500  Metric:1
          RX packets:1389219 errors:0 dropped:0 overruns:0 frame:0
          TX packets:1419096 errors:0 dropped:0 overruns:0 carrier:0
          collisions:0 txqueuelen:1000
          RX bytes:572275856 (545.7 MiB)  TX bytes:771215630 (735.4 MiB)
          Base address:0x2000 Memory:d0120000-d0140000
```

Accessing Sorcerer from non-Windows Computers

Computers on a MS- Windows network can usually refer to Sorcerer by its SAMBA name, which by default is `pe-sorcerer`.

For other computer types, or if you prefer, also from Windows computers, you need to provide Sorcerer's network name or address. This may be a static IP address as set up in Fixed IP Addresses, or it may be dynamic. To find out the IP address, type `/sbin/ifconfig` and view the report for the active Ethernet connection, usually `eth0`. Note the `inet addr` field (e.g. `192.168.1.104`) — this is the IP address you will need.

Note that dynamically assigned IP addresses are susceptible to reassignment, which may happen, for example, if either the router or the Sorcerer is power-cycled. In such cases a new number may be needed the next time.

SAMBA Setup

SAMBA is a convenient way to transfer files between a Microsoft Windows environment and a Unix-based system such as Sorcerer. SAMBA is a file sharing system where Unix can serve file systems using Microsoft Windows protocols. These file systems are then accessible on Windows clients with no configuration on the client end — they look just like Windows machines.

SAMBA is set to run by default in Sorcerer. If you have a simple network as described in Basic Installation, then no configuration is required to use use SAMBA from a PC attached to the network. If you want to change the workgroup name and/or server name, perhaps because you have more than one Sorcerer unit on the network, you can do this in the `/etc/smb.conf` configuration file. Make the changes carefully, keeping a back-up copy, and then restart the SAMBA server. To change the server name to `sorcerer-b`, for example you would change the following line in that file:

```
netbios name = sorcerer-b
```

The SAMBA server needs to be restarted after such changes, most simply by rebooting the machine.

Firewall Considerations

It is recommended to use Sorcerer together with the clients that access it behind a common firewall, which gives security from the internet or a larger institutional network, but not to use a firewall between those computers, because it may interfere with access to Sorcerer. This is how Sorcerer is configured on delivery, with the internal firewall software turned off. If the Sorcerer system is isolated from the internet, or is behind an effective separate firewall, as is usually the case in an institutional environment, there is little risk in disabling the firewall.

Stand-Alone Network Configuration

Sorcerer is designed to drop into typical networks and to be immediately functional. However, networks are complex, and pre -existing settings may in some environments get in the way of plug-and-play operation. In that case, a stand-alone network consisting just of Sorcerer and one other computer to act as a client may be needed. Such a network can be implemented either permanently or temporarily and is useful for:

- Initial set-up of Sorcerer and verifying correct operation
- Confirming or altering Sorcerer's default network settings
- Isolating network problems.

To set up a stand-alone network with Sorcerer, follow these steps:

- Use a 10/100 BaseT ethernet router with a built-in DHCP server and at least two available ports. (Such devices are common in home and small office settings for sharing an internet connection between multiple computers — a typical product is the Linksys BEFSR41 "EtherFast Cable/DSL Router with 4-Port Switch".) Make sure the router is configured, as they usually are by default, to assign IP addresses using DHCP and to allow all protocols/ports/MAC addresses.
- Locate a Windows XP or 2000 computer (a laptop may be convenient) with an available ethernet adapter to act as a client. Before plugging it into the new network, ensure that the network settings are configured as follows.

- In the Network Connections control panel, find the entry for the ethernet adaptor (e.g. "Ethernet Local Area Connection") and right-click to select Properties.
- Ensure Client for Microsoft Networks and TCP/IP are available and active in the list of available protocols
- Select TCP/IP and click Properties
- Use Obtain an IP Address Automatically. In Advanced Settings, under WINS, enable NetBIOS over TCP/IP.
- Hit OK on all dialogues to close the control panel and accept these settings.
- Power the computer down and then connect it to the router using the ethernet adaptor port using a standard RJ-45 cable.
- Attach Sorcerer's Ethernet port 0 via another RJ-45 cable to another port on the router
- Power up the router first and then the two computers.

At this point, all the devices should be set up to communicate both with TCP/IP using IP addresses automatically assigned by DHCP as well as with Microsoft Networking. You should now be able to see Sorcerer from the Windows machine as described in the section Initial Setup of Sorcerer 2 Tower/Rack and Solo.

Configuring and Updating Sorcerer Software

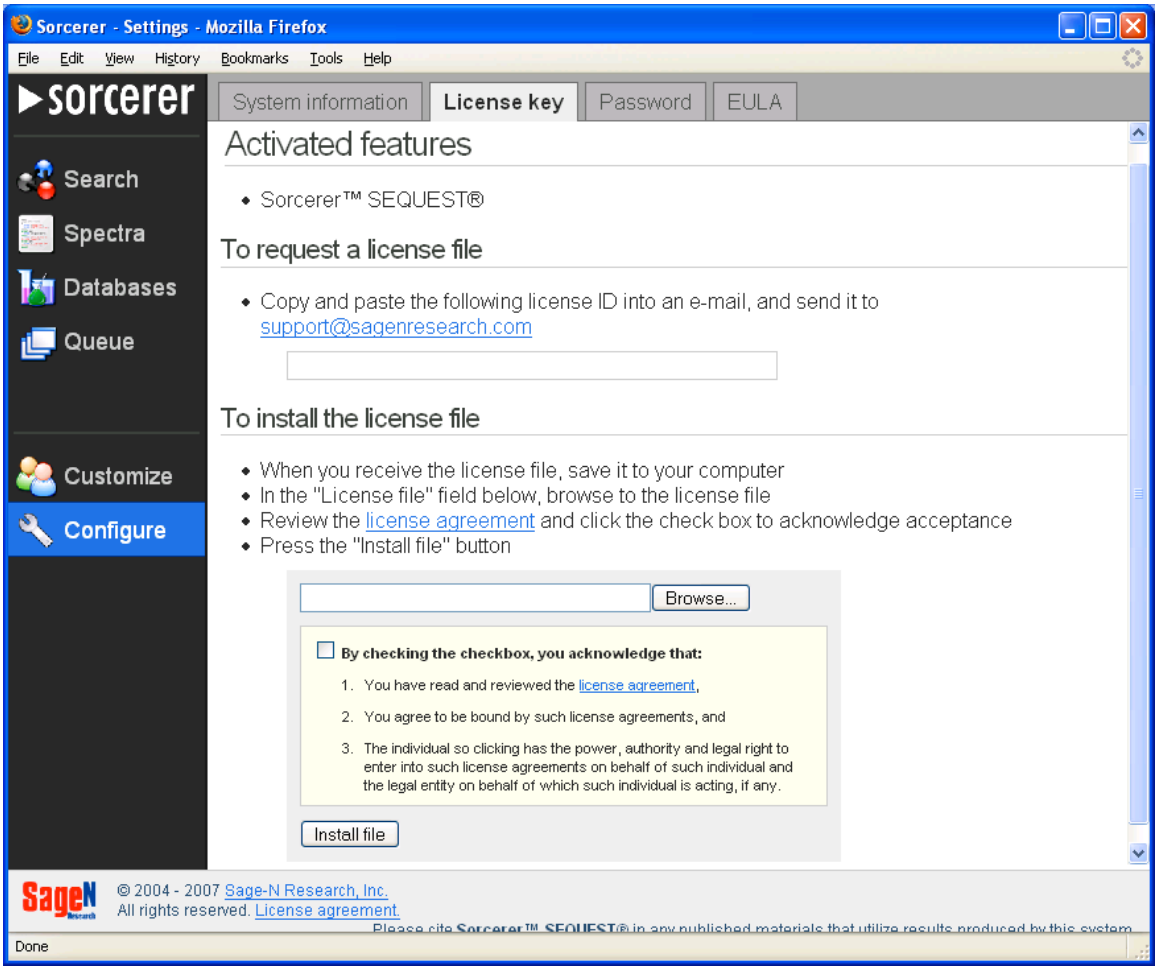
Entering Software License Keys

Sorcerer generally requires one or more software license keys in order to operate. The Sorcerer PE license key is needed to to use the Sorcerer tools, including SEQUEST searches. To use Scaffold and the integrated Scaffold Batch program that is available either separately or bundled with Sorcerer, a separate Scaffold Batch license key is required. It is apparent from the Sorcerer Web GUI when you try to use these functions if the licenses are not activated.

Please note that newly delivered and evaluation systems are supplied with temporary 30-day license keys. These should be updated with the permanent keys when you pay for a purchased system. In this case, please contact support@sagenresearch.com for the key codes if you have not already received them. You will receive the codes by email; please save them and enter them as described in the following sections.

Entering a Sorcerer PE License Key

This can be done from the Sorcerer Web GUI. Click Configure on the Toolbar, and then click the License Key tab. Follow the instructions on that page.



The terms under which the license is provided are accepted when you first start using the system, and are viewable by clicking the EULA tab.

Entering a Scaffold Batch License Key

Scaffold Batch is generally preinstalled on new Sorcerer shipments. If it has not already been installed, or if a new version of Scaffold Batch is suggested by Sage-N Research, then please install it as described under Installing Scaffold and Scaffold Batch. Usually, installing a new version does not require a new license key.

If the program requires a valid key, it will prompt for one when it starts up, and the user can enter it. The system must be have Internet access, with DNS available, for the license to be activated (it need not be kept on the Internet once activated).

The key can be entered either in the graphical UI of Scaffold, or in the command line interface of Scaffold Batch. A key valid for Scaffold Batch can still be entered in the interactive version of Scaffold and Scaffold Batch will be enabled if the license key is valid for it.

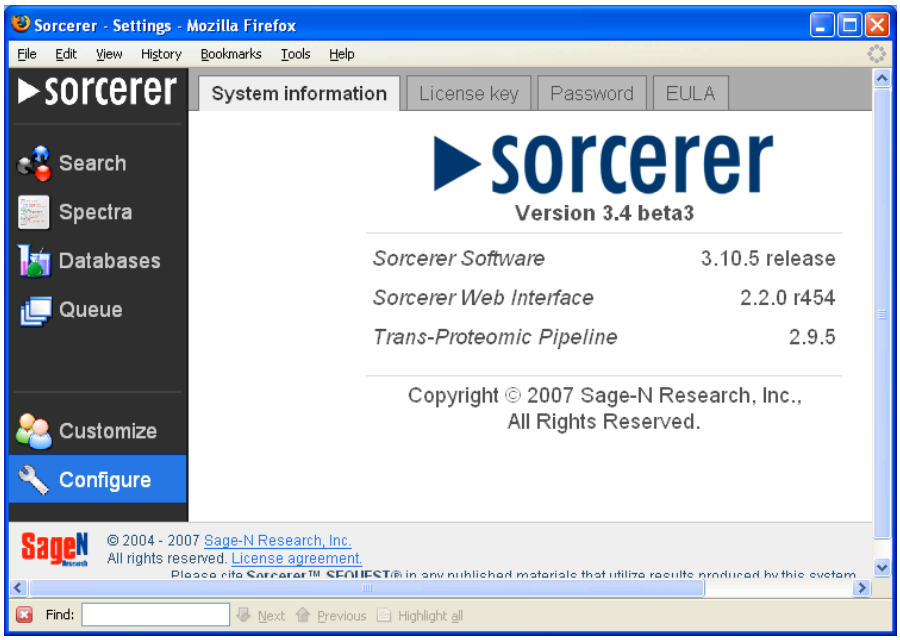
To start the program and enter the key, log in to Sorcerer as the `sorcerer` user and choose one of the following two methods:

- Start the Linux Gnome desktop as described in Linux Desktop Tools and select Scaffold from the Applications menu, or
- At the Linux command line (either logged in locally or over the network), type `ScaffoldBatch2`

In either case, enter the key when prompted.

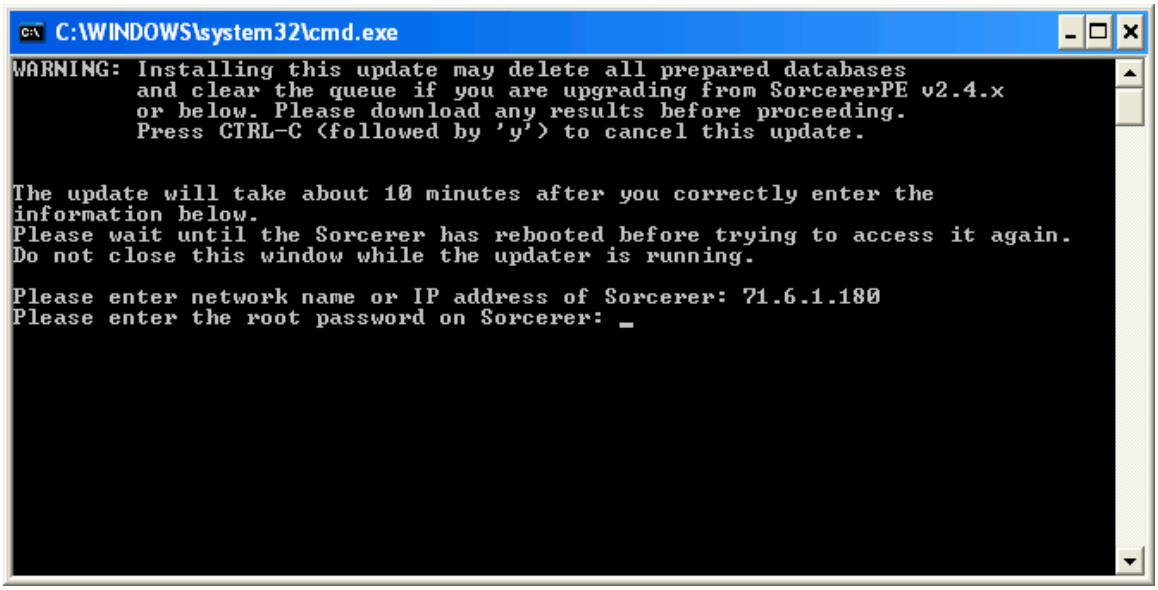
Software Updates

The version number of the currently installed software can be checked by going to Configure Sorcerer / System Information in the Sorcerer Web GUI. The primary Sorcerer PE version number is listed, along with versions of some of its components.



Sage-N Research generally supplies updates as an executable file for Windows, which connects from the PC it is running on to the Sorcerer system, and runs scripts to update the Sorcerer. First, read the release notes that accompany the update. To use the updater, follow these general steps (depending on the update, there may be minor variations):

- Download or copy the updater .exe file to a Windows computer that can currently access the Sorcerer GUI.
- In Windows Explorer, double-click that file.
- It will open an MS-DOS command prompt window, and will prompt for items such as the Sorcerer network name/IP address and account passwords. Type in these values and press Enter after each prompt.



- Messages will scroll by showing progress with the installation. Allow these to complete without interruption, and take note of any final error messages.

```
sorcerer_software-v3.4.tg |      63836 kB | 3546.4 kB/s | ETA:
00:00:20 |  46%
```

```
reboot
Press any key to continue . . .
```

- To complete the install, Sorcerer will usually reboot itself. Allow 2-5 minutes for the reboot, and then check the new version number in the GUI.

Note that some major upgrades may need to remove databases or other user data, which will need to be restored after the update. If this is the case, the release notes will say so. In any event, it is wise to back up user data before updating the system — see Backing up Data.

Using Sorcerer

Moving Files to and from Sorcerer

There are three convenient ways to move files, such as spectra data files, databases, and results, to and from Sorcerer. The first is to use the Sorcerer Web GUI, which lets files be uploaded or downloaded in context-specific ways when those files are being selected. Another way is to use the Linux commands or the Gnome User Interface to move files within the file system of Sorcerer. Finally, when using Sorcerer as a Windows file server, you may drag and drop files in Windows Explorer.

Which method is best may depend on what computer you are using for the operation and the type of data transfer you are doing. Thus the Web GUI can be used from any computer on the network, and requires no set-up on the client, but it can be slow, especially for large files like sequence databases. Linux tools can only be used for moving files that are already on the Sorcerer itself. The Windows Explorer approach is suitable for transferring files across the network from Windows clients.

Uploading and Downloading Files in Sorcerer GUI

The Web GUI has built-in facilities for transferring files that Sorcerer takes as input and generates as output. There is an upload tool in the File Browser for selecting spectra data and FASTA sequence databases when those files are needed. There are also links for from a finished search in the Queue View.

To upload files, press Upload in the file selection window, and a file entry field with two buttons (Browse… and Upload File) appears. You can either type into that field, or press Browse… to choose a file on the local PC to be uploaded. Select it, and the field will reflect the name. Now press Upload file to initiate the file transfer. If it is a big file, be patient while the transfer proceeds — there is no feedback from the browser.

To download files, select the Download Results tab in the Search Results view. To download zip archives of the results files, set the checkboxes for the desired files, then press the

button for the save or open dialogue. For Scaffold files, simply click the link.

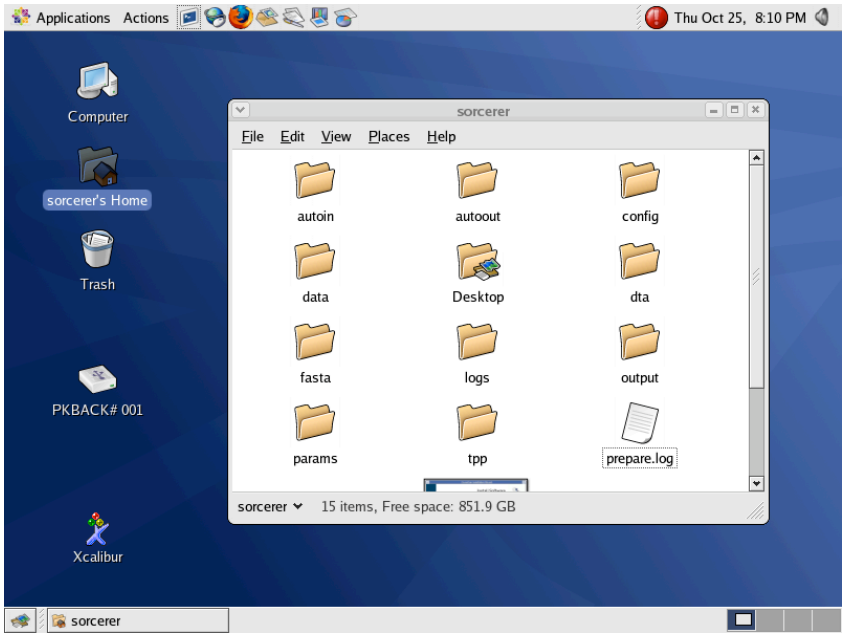
Notes and caveats:

- A transfer of large files or lots of files can take a long time, and due to limitations in the web technology, there is no indication of progress. You can however check file sizes in Windows Explorer to see what's happening.
- Again due to limitations in the technology, the browser can only select a single local file for upload, but this may be a zip archive containing multiple files.
- It is very inefficient (even if it's handy) to use the Web to transfer files that are already on Sorcerer itself (say to move a FASTA file which you have already downloaded into Sorcerer's `sorcerer/fasta` directory). That's because the data transfer has to go through the client computer.
- Zip archives that are uploaded are automatically extracted into the current directory by Sorcerer. This is useful for sets of spectrum files, for example, and gets around the problem of transferring multiple files.

Moving Files within Sorcerer Using Linux

This is the best approach for moving files that are already on the Sorcerer within the Sorcerer file system. For example, if you download a Fasta file over the internet to be installed for Sorcerer searching, it's best to move it to the `sorcerer/fasta` directory from the desktop (or wherever it was downloaded to) using Linux tools, rather than the Sorcerer Web GUI, which needs to treat it as a network transfer (inefficient), even although the file is already on the Sorcerer system.

To use the file manager in the Linux Desktop, click on the `sorcerer` home directory icon, and then on `data`, or `fasta`, or whatever directory you are using. Drag and drop the files to be transferred onto or from these folders.



You can also use this method to transfer files to and from CD-ROMs and USB memory sticks. Simply insert them, and they will show up on the desktop. Double-click the icons to display their contents, which you can drag and drop to and from Sorcerer folders. When you have finished with the devices, right-click them to unmount them or eject them.

Using SAMBA to Transfer Files

This is a simple way to drag and drop files using Windows Explorer or a file selection dialog in another Windows program. SAMBA makes Sorcerer look like just another Windows server on the network. It is best, particularly when using Bioworks, to set that up as a mapped network drive before you start.

See Using Sorcerer in a Windows Environment above for how to set up a SAMBA share, and how to set up a mapped drive for convenient future access.

Now you have an easy way to move files such as protein sequence databases, spectra and search results between the two systems by dragging and dropping to this network drive. However, be aware that this can be very slow when dealing with lots of little files, such as thousands of DTA files, and it is more efficient to transfer them as a single zip archive and extract them at the destination.

Starting and Stopping Sorcerer

To start Sorcerer, first connect it to the network, power and any peripheral devices as described in Initial Setup. Then the unit may be powered up by pushing in the power button on the front panel. When Sorcerer starts up, it automatically starts up all the services required to use and operate the Sorcerer software, including the Web server for the graphical interface and a SAMBA server for file transfer. The entire sequence may take a couple of minutes to complete.

It is not necessary in routine operation to shut Sorcerer down. One of the following circumstances may however call for a controlled shut-down:

- To change the hardware or network configuration of Sorcerer
- To move or ship Sorcerer
- To reset the system following a transient failure

To shut Sorcerer down, use one of these two methods:

- At the commandline, as root, type `/sbin/poweroff`
- In the Linux Gnome desktop, choose Shutdown from the Logout menu.

Depressing the power button for several seconds will also power the unit off without going through the shutdown sequence. It is recommended not to use this method while Sorcerer is running because it is possible that files and data can be corrupted.

Disk Management

Sorcerer has a substantial amount of internal disk space that is used for the following items:

- Operating Platform (OP) and Linux files – throughout the filesystem in / and its subdirectories
- Sorcerer application software – mostly in `/usr/local/SageN`
- The MySQL-based database
- User files in the following directories:

- `/home/sorcerer/data` — spectra files, including .srf, .mzXML, .mgf and .dta files
- `/home/sorcerer/output` — search results, including .out files, Scaffold .sfd files and TPP files. Each subfolder corresponds to a different search.
- `/home/sorcerer/fasta` — sequence database files in .fasta format

Cleaning up Search Output

Searches can generate a lot of output data, especially if postprocessing in tools like TPP is selected. Deleting a search entry from the queue will delete all the associated results data.

Cleaning up User Files

The OP and Sorcerer application software files are essentially fixed, but the user files in `/home/sorcerer` and the contents of the database will grow with usage of the system. It may become necessary to clean up extra files to make room for new ones. If the file systems become completely full, it can lead to failures in database preprocessing or Sequest searches that may not be completely obvious at first glance. To get a general sense of the disk usage, look at Database Administration in the graphical user interface.

To clean up sequence databases using Sorcerer's Web GUI, follow these steps:

- Select Configure Sorcerer from the toolbar
- Select Database Administration
- Check the Protein and/or Peptide Databases you wish to delete. (As a reminder, peptide databases for searching are derived from protein databases that typically correspond to protein databases. There may be more than one peptide database for each protein database. Typically, you shouldn't delete a protein database unless you delete all peptide databases that are derived from it. Also, the bulk of the disk space goes to the peptide database.)
- Press Delete Selected

- You can also delete the associated FASTA database in the `/home/sorcerer/fasta` directory once all derived peptide databases are removed, but not before.

Backing up Data

Sorcerer is not intended for archival of critical data. Despite robust engineering and RAID technology, disks and other hardware can fail, data corruption can occur and, in a multi-user environment, users can inadvertently remove or spoil one another's data. You are advised not to place the sole copy of your spectrum data on Sorcerer, and it is recommended to copy your search results from the system when searches complete, either by downloading them from the Sorcerer GUI, or by copying them from the appropriate numbered folder in the output directory.

Configuration Troubleshooting

This section presents some tools and techniques for diagnosing and fixing problems that may arise while configuring Sorcerer systems as described earlier in this document.

Troubleshooting a standard network setup

Here are some tips for diagnosing and addressing possible problems with the standard basic network set-up.

- As a general rule, if you have changed anything in the network configuration on Sorcerer, any client or a router and it is not working properly, reboot everything in the sequence: router, Sorcerer, client.
- If you continue to have networking issues, then there may be interference from the existing network. Set up a stand-alone network as described under Stand-Alone Network Configuration, at least until any issues have been identified and addressed.
- If Sorcerer is not showing up using SAMBA in Windows Explorer or if using that name in the Web GUI does not work, then either explicitly search for a computer named `sorcerer-pe`, or wait 10-20 minutes for broadcast messages from Sorcerer to take effect on the network. (Generally the name takes effect in the Web GUI immediately.)
- If you still cannot access Sorcerer by that name, then perhaps you have changed it, or SAMBA is not working properly – see Troubleshooting SAMBA Issues below. However, you will still need to access Sorcerer somehow, and if you cannot use the SAMBA name you will need the IP address.
- To figure out a dynamically assigned IP address, use the status view of your router. If you have a command line connection to Sorcerer, look for the `inet addr` field when you type:

  ```
  $ /sbin/ifconfig eth0
  ```

- You can use this IP address (192.168.0.2, for example) from your client in a variety of ways to access Sorcerer. A full description of Microsoft networking tools is beyond the

scope of this document, but the following tests may be useful:

- `ping 192.168.0.2` — to see if Sorcerer is apparently on the network at all
- Use PuTTY for a secure shell connection — to connect at the command line
- Enter `http://192.168.0.2/` in the web GUI — to see if the Web server is working properly

Troubleshooting SAMBA Issues

If the `sorcerer-pe` server fails to appear in Windows Explorer as described under Using SAMBA to Transfer Files, or if you are unable to use the name to access the graphical user interface, it may be because the SAMBA server is not running. To get the server running, you need to login as root and take the following steps:

- Check to see if SAMBA is running already by seeing if the system lists the process when you type the following

```
# ps -ef | grep smbd
```

- To start the SAMBA server if not

```
# /sbin/service smb start
```

- To set it up so that it runs automatically next time you reboot

```
# /sbin/chkconfig --level 35 smb on
```

If you see the server, but you find that access is denied, it may be because the by-default-enabled Fedora firewall interferes with the connection. In this case, you may have to disable it.

If you see the server, but you cannot log in (and the user name prompt keeps re-appearing) it may be because you do not have an authorized log in. There should be the user name / password combination of `sorcerer/sagen` set up by default, but if it needs to be restored, it can be done using the `smbpasswd` command. For example, to add this name and password, do this:

```
# smbpasswd -a sorcerer
New SMB password: sagen
Retype new SMB password: sagen
... Added user sorcerer.
```

A full description of SAMBA configuration is complex and well beyond the scope of this document. Non-standard configurations cannot be supported by Sage-N Research, Inc.

Troubleshooting Firewall Issues

If you get access denied messages or attempted connections that time out, especially if it happens only with some protocols, suspect firewall settings, either in a router or in Sorcerer. At least temporarily, set up a stand-alone network as described above, and turn firewalls off.

Troubleshooting Application Software Issues

The software has been engineered for flexibility, robustness and performance, but occasionally it may not behave as expected. It is impossible to predict specific failure conditions, and therefore to give specific recovery instructions. General strategies for diagnosing, working around and reporting apparent software failures are similar to most other packages and include the following approaches:

- Observe error messages, note settings and save input and output files in case a problem needs to be reported
- Review the log file for errors and unusual conditions, by following the chart icon in the Queue View in the Sorcerer Web GUI. (Note that this information will also generally be requested by Sage-N Research technical support staff when their assistance is wanted.)
- Ensure enough system resources are available. Sorcerer is data-intensive so ensure disk space is available, using the techniques in the section on Disk Management.
- Is the system busy? If you are comfortable with using the Linux tools, or in consultation with Sage-N Research technical support, see if the CPU is busy, files are being written, etc.
- If an operation fails in the graphical interface, try the command line equivalent.
- Is the problem reproducible? What happens if you try again? Does the problem still exist if you power-cycle Sorcerer?

- Clean up partial results and try again. Perhaps choose new names for objects if there is a conflict. Avoid punctuation symbols and white space in objects' names.
- Try a very simple search, using a small spectrum set, a default search profile, and a standard database, such as SwissProt.

If the problem remains, there are four main likely scenarios:

- Your search is too big or complex. The quantity of spectra, parameters that are too unconstrained and the size of the peptide database can cause this, as well as complex post-processing requests.
- The software configuration is damaged. It is likely that the attempted operation (search, database processing, etc.) will fail no matter what the data set and settings are, even a basic one. In such a case, the software may need to be repaired or completely re-installed. Contact Technical Support for assistance with this task.
- There is a hardware failure causing a software failure indirectly. See Hardware Troubleshooting below.
- You have encountered a bug in the software. Since the software is tested on release on a variety of test sets, the bug is likely to be specific to your datasets and search parameters. Please contact Sage-N Research Technical Support to report the bug and to receive advice on further diagnosis, work-arounds and software fixes. The more information you can provide in terms of input data, output, settings and messages, the easier it will be to reproduce the problem and to give effective advice. At a minimum, please supply the log file for a search or a database preparation. This can be found using the 'chart' icon in the entry for that job in the Queue View of the GUI.

Hardware Troubleshooting

If a hardware malfunction is suspected, first note or save all messages and information in case it is required for a problem report. Then completely power down the Sorcerer (not just rebooting, but switching it off entirely), and then power it back up. (Sometimes this cures transient failures.)

In the case of a confirmed persistent hardware malfunction, the unit may require a return to the supplier for a replacement.

Returns must be authorized by a Sage-N Research representative prior to shipment, in accordance with Sage-N Research's RMA procedure. The unit will be repaired or a substitute unit will be provided. There are no user-serviceable components in the system and opening the unit or any attempt to manipulate the internal components may compromise the system and will void any warranty that may be in effect. It may also create a safety hazard or the possibility of electric shock to expose the internal components.