

Spartan '04 Server for Linux

Installation of Spartan '04 Server from CD-ROM

Insert and mount the CD-ROM.

As root user perform the following steps.

RedHat/Fedora Linux:

```
cd /mnt/cdrom
./spinstall.sh
```

SuSE Linux:

```
cd /media/cdrom
./spinstall.sh
```

The installation program will unpack and install the correct version for the system Spartan is being installed on. Spartan '04 has three separate versions to support both 32-bit and 64-bit processors. The 32-bit version supports Intel Pentium III, Intel Pentium 4, Intel Xeon, Intel Pentium M, AMD Athlon, and AMD Opteron. There are two 64-bit versions. The first 64-bit version supports Intel EM64T (newer versions of Intel Xeon and Pentium 4) and AMD64 (AMD Athlon64 and AMD Opteron) processors. This version will only be installed on operating systems which provide support for 64-bit processors. The second 64-bit version supports Intel Itanium processors.

The installer will prompt for the directory where Spartan is to be installed. This allows flexibility in placing the Spartan executables in a directory with sufficient disk space. This also allows the Spartan executables to be installed on a network storage server. Spartan can then be installed on additional systems that have access to this network storage by running the following abbreviated installation...

```
cd /usr/spartan04.123_2[46]_int{8,8e}
(“/usr” is the default, substitute the directory chosen during the installation)

./sp_install
```

This installation method skips the unpacking of the Spartan executables and simply configures Spartan for the local system.

After the installer has unpacked Spartan onto the system, a series of questions will be asked to configure Spartan.

```
Queue type?
Scratch storage location?
Scratch limit per job?
Memory limit per job?
Access Code?
```

Queue Type?

There are two choices for queuing, internal and external. Select internal to use the queue that is built into Spartan. It is a simple FIFO (First In First Out) queue. It is useful on standalone systems that don't have any other queuing capability installed. If a queue is available (e.g. OpenPBS, Torque, LSF), select external. This will result in Spartan submitting jobs to a queue that is external to Spartan.

If internal is chosen, the “*Maximum number of running jobs*” will be prompted for. This number defaults to the number of processors in the system. Accepting the the default should work fine unless the processors support hyper-threading. In this case the number of processors will be double the number of physical processors. Override the default and enter the number of physical processors.

Scratch Storage Location?

Some higher level Spartan jobs require the use temporary disk space. Enter a directory where sufficient disk space is available.

Scratch limit per job?

Specify the amount of disk space available per job. Take into account the number of running jobs allowed by the queue. The minimum recommended amount of disk space per job is 20000MB (20GB). Larger amounts of disk space will help with higher levels of theory (MP2,MP3...).

Memory limit per job?

Specify the amount of physical memory (RAM) available per job. Take into account the number of running jobs allowed by the queue. The installer will attempt to determine the amount of memory and apply a formula to calculate the amount of memory per job. The minimum amount of memory required per job for good performance is 512MB. The recommended amount of memory per job is 1024MB.

Access code?

An access code is required to run Spartan on each system. The installer will present a set of 12 hexadecimal doublets which uniquely identifies the system. These doublets must be e-mailed to Wavefunction at access_codes@wavefun.com. The unique identifier will be used to generate an access code that will activate Spartan '04 for this system. Access codes can be administered from outside the installation process. This allows the installation to be completed and the access code to be entered at a later time with the command...

```
spartan --setup
```

Configuring Spartan '04 server to accept job requests from a Windows client

Spartan '04 Server makes use of the Samba Server to accept job requests from Windows PC clients. Two resources are needed to accept jobs. A file share and a pseudo printer.

When a PC client submits a job to the server, it first copies a Spartan Document to a file share on the server. Then the client sends a print request to the server. The print request is simply a file that contains the path to the Spartan Document on the server. The pseudo printer launches Spartan which processes the Spartan Document performing any requested analysis on the molecules contained in the Spartan Document. When the job is finished the PC client copies the Spartan Document back to the PC and the user is prompted with a job completion message.

A file-share and pseudo-printer are configured by editing the samba configuration file...

```
/etc/samba/smb.conf
```

Adding the following section to the samba configuration file will make the directory “/spartan_Share” available to users *andy* and *phil* on hosts *volvo* and *ferrari*.

```
[Spartan Share]
  comment = Spartan Share
  path = /spartan_share
  valid users = andy phil
  read only = No
  hosts allow = volvo.wavefun.com ferrari.wavefun.com
```

Typically the directory “/spartan_share” should be world-writable with the sticky bit set. The directory can be created as follows...

```
mkdir --mode 1777 /spartan_share
```

Also, users *andy* and *phil* will need an entry in the `/etc/samba/smbpasswd` file. The SMB password used for each user must match their password on the Windows client. A password entry can be added by the root user by running...

```
smbpasswd -a andy
```

After the entry is added, users can update their SMB password by running...

```
smbpasswd
```

Test the file-share by copying a file from a Windows client to the file-share. The file should be copied without requesting a password.

Next, add the following to the samba configuration file to enable a pseudo-printer. Un-comment the directive “printing = sysv” for Samba version 3.0 or later.

```
[spartan]
    comment = Spartan
    path = /var/spool/spartan
#    printing = sysv
    printable = yes
    print command = /var/spartan/spartan_samba %s
    browseable = yes
    guest ok = no
```

Again, typically the directory “/var/spool/spartan” should be world-writable with the sticky bit set. The directory can be created as follows...

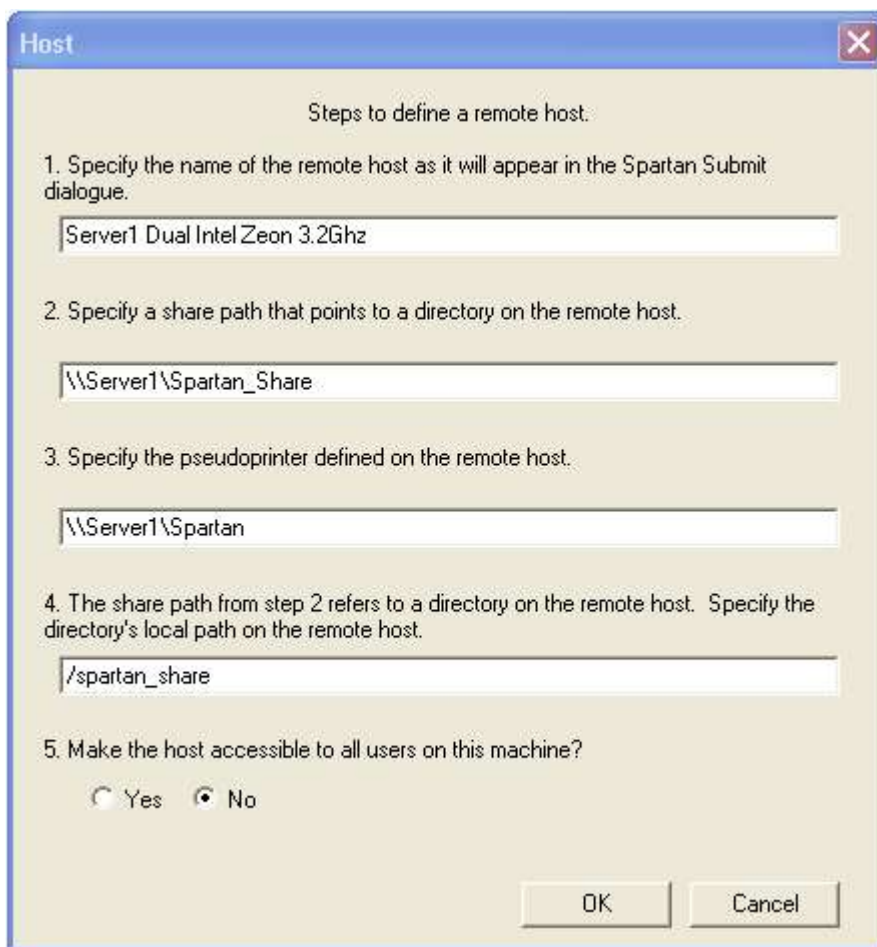
```
mkdir --mode 1777 /var/spool/spartan
```

The server is now configured to accept jobs from a Windows client. The next step is to configure Spartan on the Windows client to submit jobs to the server.

Configuring a Windows Client for remote submittal of jobs

Submitting jobs from a Windows client to a Linux server requires Spartan '04 version 1.0.3 for Windows. This version contains the functionality required to interact with Spartan '04 Server for Linux. A dialog panel to configure Spartan '04 for Windows for remote submittal can be accessed by selecting *Preferences* from Spartan's *Options* pull-down menu, and then selecting the *Hosts* tab.

The Preferences/Hosts Panel allows for the addition, modification, and removal of servers to which jobs can be submitted. Select *New...* to add a server to the list. Five input fields will be presented. The first field is for descriptive purposes only, so enter something that describes the server (e.g. Name, Manufacturer, Processor Speed). The second field specifies a file share that the user can access on the server. This file share is where the Spartan molecule file is copied prior to starting a job. The third field specifies a pseudo printer which will be used to start the job on the server. The fourth field specifies the path of the file share as seen from the server. A fifth entry is activated only if the user is an administrator. Selecting *Yes* will make this entry available to all users on the Windows system. Below is a sample of the host definition dialog.



Spartan is now configured to submit jobs to a remote server. The next time a job is submitted an additional panel will be presented which will allow the selection of the server to run the job on. For the case of a new unsaved molecule, the *Save As – Submit* dialog will have an additional menu titled *Submit To*.

Files created during installation

The installation program will create the “/var/spartan” directory to contain several configuration files. The files created are:

/var/spartan/spartan	Spartan run script
/var/spartan/spartan_samba	Spartan Samba run script
/var/spartan/queue_entries	Spartan internal queue
/var/spartan/queue_limits	Spartan internal queue attributes
/var/spartan/sp_access	Spartan access codes
/var/spartan/qchemrc	QChem resource directory

The installation program will also create the symbolic link...

```
/usr/bin/spartan -> /var/spartan/spartan
```

The link is created to conveniently place the Spartan run script in the search path of all users. This allows users to access Spartan without having to augment their search paths.

Removing Spartan '04 Server

Spartan does not have an “un-install” script, but removal of Spartan is quite simple.

```
rm -r /usr/spartan04.123_2[46]_int{8,8e}
(“usr” is the default, substitute the directory chosen during the installation)
rm -r /var/spartan
rm /usr/bin/spartan
```

Note: If the intention is to remove Spartan '04 and replace it with a newer maintenance release, skip the last two remove commands (rm) listed above. This will preserve the access codes and the settings entered during the previous installation.