Spartan '06 for Linux Installation Instructions

Section 1. <u>Installation from CD-ROM</u>

Insert and mount the CD-ROM.

As root user perform the following steps.

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

There are 3 separate versions of Spartan'06 for Linux: a 32-bit version supporting Intel Pentium III, 4, Xeon, M, and AMD Athlon; a 64-bit version supporting EMT64 (newer versions of Intel Xeon and Pentium 4) and AMD64 (Athlon64 and Opteron); and a second 64-bit version for Intel Itanium processors. The installation program will unpack and install the appropriate version for your system.

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/spartan06.129_26_int{9,9e}
```
   ("/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?
There are two choices for queuing, internal and external. Select internal to use Spartan's integrated queue. This is a simple FIFO (First In First Out) queue, and is useful on standalone systems that don't have other queuing capabilities 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 is appropriate 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.

Remote Job Storage Location?
This is the directory where jobs submitted from remote systems will be stored. Typically this directory should be world-writable with the sticky bit set. The sticky bit should be set such that only the owner of a job is allowed to delete or rename the job. The default choice is "/tmp" which is world-writable with the sticky bit set.

Scratch Storage Location?
Some higher level Spartan jobs require the use of temporary disk space. Enter a directory were sufficient disk space is available. Typically this directory should be world-writable with the sticky bit set. The sticky bit should be set such that only the owner of a scratch file is allowed to delete or rename it. The default choice is "/tmp" which is world-writable with the sticky bit set.

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 identify 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 '06 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
```

Section 2: Installing the Spartan Database from DVD-ROM

Insert and mount the Spartan Molecular Database DVD-ROM.

The DVD-ROM contains three directories that make up the Spartan Database, Small Molecules, Ligands and Reactions. These three directories must be copied to the directory where Spartan was installed.

```
cd /usr/spartan06.129_26_int{9,9e}
```

> *"/usr" is the default installation directory, substitute the directory chosen during the installation performed in Section 1.*

```
cp -r --preserve=mode /media/cdrom/Small\ Molecules .
cp -r --preserve=mode /media/cdrom/Ligands .
cp -r --preserve=mode /media/cdrom/Reactions .
```

> *This assumes the DVD-ROM is mounted under "/media/cdrom"*

The three directories require ~3.2GB of storage so be sure adequate disk space is available.

Section 3. Accepting job requests from a Linux client

Spartan '06 makes use of *ssh* and *scp* to to accept job requests from a remote Linux client.   To make use of *ssh* and *scp*, Spartan requires the ssh server allow the client to have access without prompting for a password or passphrase. This can be arranged in several ways. The easiest is to use public key authentication.   The instructions on how to setup public key authentication follow...

On the Linux client...

```
ssh-keygen -t dsa -N '' -f $HOME/.ssh/id_dsa
```

This command will generate two files. The file "`$HOME/.ssh/id_dsa`" is the private key and the file "`$HOME/.ssh/id_dsa.pub`" is the public key.

Copy the public key file to the server (replace *server* with the name of your server).

```
scp $HOME/.ssh/id_dsa.pub server
```

On the Linux server...

```
mkdir $HOME/.ssh
cat $HOME/id_dsa.pub >>$HOME/.ssh/authorized_keys2
```

Test the configuration from the Linux client...

```
ssh server
```

You should not be prompted for a password or passphrase, and should simply be presented with a shell prompt.

Section 4. <u>Configuring a Linux Client for remote job submittal</u>

By default, Spartan submits jobs to the local system. To configure Spartan to submit to a remote system, access the *Preferences* dialog found under the *Options* menu in the Spartan Graphics User Interface. Now select the *Hosts* tab. To add a new host select the *New* button. Existing entries can be managed by selecting the *Edit* or the *Delete* buttons.

A good way to test the configured hosts is to run the Spartan monitor. The monitor probes a remote system by using *ssh*. Since remote job submittal also requires the use of *ssh*, the monitor provides a good initial check to see if *ssh* is configured correctly.

The monitor can be accessed from the Spartan Graphical User Interface by selecting *Monitor* from the *Options* pulldown menu. The monitor will probe each configured host and produce a listing of Spartan jobs found. Note: By default, the monitor only probes the local system. To make the monitor probe remote systems, select "Filters" from the monitor's "View" menu. Select "All" for "Hosts:" and then select "Done". The monitor will now probe each of the systems configured in the hosts file.

Section 5. <u>Accepting job requests from a Windows client</u>

Spartan '06 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 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, 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
```
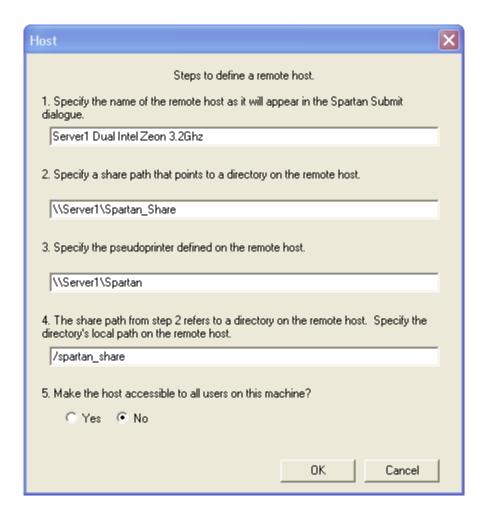
The server is now configured to accept jobs from a Windows client. The next step is to configure Spartan on the Windows client to submit jobs to the server.

Section 6. <u>Configuring a Windows Client for remote job submittal</u>

Submitting jobs from a Windows client to a Linux server requires Spartan '06 for Windows version 1.1.0 of later. This version contains the functionality required to interact with Spartan '06 for Linux. A dialog panel to configure Spartan '06 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 were 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.

Host

Steps to define a remote host.

1. Specify the name of the remote host as it will appear in the Spartan Submit dialogue.

> Server1 Dual Intel Zeon 3.2Ghz

2. Specify a share path that points to a directory on the remote host.

> \\Server1\Spartan_Share

3. Specify the pseudoprinter defined on the remote host.

> \\Server1\Spartan

4. The share path from step 2 refers to a directory on the remote host. Specify the directory's local path on the remote host.

> /spartan_share

5. Make the host accessible to all users on this machine?

> ○ Yes   ● No

[OK]   [Cancel]

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*.

Section 7. <u>**Files created during installation**</u>

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/spartan_ssh          Spartan Ssh run script
/var/spartan/remote_job_path      Path to store remote jobs
/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.

Section 8. <u>**Removing Spartan**</u>

Spartan does not have an "un-install" script, but the removal of Spartan is simple.

```
rm -r /usr/spartan06.129_26_int{9,9e}
("/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 '06 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.