QUANTA

Administration Guide

MARCH 2006

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Contents

Installation & Administration Guide

Note: The most current version of these notes is maintained at the QUANTA 2006 website:

http://www.accelrys.com/doc/life/QUANTA2006/

If you are reading this from a CD installation, or a printed or older downloaded copy, this may not contain the most complete information.

This book is for licensees of QUANTA 2006.

To install QUANTA 2006 you should be familiar with basic UNIX® commands and shell environment variables. The examples in this book presume that the C-shell is in use.

If you are installing into a networked environment, the network should be installed, tested, and running before you install this software. Complex installations with multiple license servers may require additional experience with TCP/IP utilities and NFS.

Note: The CNX environment must be initialized before running CNX. To do this, you should add a line to the file exec/cnx.bat to source the appropriate resource configuration file to initialize the CNX environment.

Note: If QUANTA is installed in a directory which has a lengthy path (> ~80 characters), some calculations may fail because the path to the parameter file gets truncated. Be sure to limit path length.

QUANTA Required Software Packages

This page summarizes what software packages need to be installed on the customers system in order to run QUANTA.

Platform	Application(s)	Package Name	Description
Linux, IRIX	compress, uncompress	Linux: ncompress	Needed to uncompress and process .Z input files.
Linux, IRIX	gzip, gunzip	Linux: gzip	Needed to uncompress and process .gz input files.
IRIX	TrueColor mode		See Configuring SGI to run in 24 bit TrueColor mode (page 26)
Linux, IRIX	MolScript 2.1.2		Needed if you plan to read in MolScript files produced by QUANTA. Download from http://www.avatar.se/molscript/.
Linux	XFree86	XFree86-*	X-Windows environment on Linux
Linux	GNOME	gnome-*	Basic windowing environment needed to run QUANTA
Linux	NVIDIA drivers and OpenGL libraries		Drivers and OpenGL libraries for supported graphics cards supplied by NVIDIA at http://www.nvidia.com/content/drivers/drivers.asp. Needed for high-performance rendering of OpenGL objects.
Linux	Mesa libraries	Mesa	Libraries needed for rendering OpenGL graphics.
Linux WS 3.0 only	OpenMotif compatibility libraries	openmotif21	Libraries needed for rendering some graphical widgets.
Linux WS 2.1 only	OpenMotif libraries	openmotif	Libraries needed for rendering some graphical widgets.
Linux WS 3.0 only	C++ Compatibility libraries	compat-libstdc++	Compatibility libraries needed for running applications on WS 3.0.
Linux	GhostView 3.5.8	gv	User-friendly interface to GhostScript used for viewing PostScript files generated by QUANTA. Downloadable from http://www.rpmfind.net/. Note use the “gv” RPM and not “ghostview”.
Linux	GhostScript	ghostscript	Back-end scripting software for viewing PostScript files
IRIX	xpsview		Interface to view PostScript files on SGI IRIX.
Linux	ImageMagick	ImageMagick	Image viewing program used to take screen shots and display them.

Platform requirements

QUANTA requires the following minimum configuration on Linux:

- 1 GHz Pentium III or higher (32-bit Intel-compatible CPUs only).
- 512 MB RAM.
- Red Hat Enterprise Linux WS 3.0 or WS 4.0 running the Gnome/Sawfish desktop environment.
- Nvidia Quadro4 980 XGL graphics card using Nvidia Linux drivers.

- Background jobs can be run on servers without the graphics requirements listed above. The other hardware requirements must be met.
- Screen resolution of 1280 x 1024.
- Disc space: 300MB.

  An additional 480MB is required for database.dat (on a separate CD).
- A three-button mouse is required (for the IBM Thinkpad a *separate* three-button mouse is required).

QUANTA requires the following minimum configuration on IRIX:

- SGI IRIX 6.5.24 to 6.5.28.

  The patches required for SGI workstations are included on the QUANTA CD-ROM. Information on these patches is in the file /CDROM/platform_gifts/sgi/README.
- 512 MB RAM.
- Screen resolution of 1280 x 1024.
- Disc space: 270MB.

  An additional 480MB is required for database.dat (on a separate CD).

Note: The IRIX version of QUANTA has been tested only on 64-bit machines. This is due to the limitation that CHARMm 32b1 is only available on 64-bit machines. All newer IRIX machines are 64-bit.

1. Before you Install

Selecting an installation procedure

This book describes the complete installation procedure twice, from two points of view. You can choose to follow either the standard installation, or the manual installation procedures.

Standard installation

The majority of readers should follow the standard installation procedure described in Chapter 2. The standard installation makes use of installation scripts to automate the editing of setup files.

Manual installation

Follow the manual installation procedure described in Chapter 3 only if you have extensive experience with UNIX system administration tasks. The manual installation is appropriate for readers who are:

- Accomplished system administrators who prefer to directly edit setup files without the assistance of installation scripts
- Wary of automated installation scripts, and want to learn more about the scripts before running them

For either installation procedure

Read the rest of this chapter regardless of the installation procedure you select.

Hardware and operating system requirements

QUANTA 2006 is supported under:

- SGI IRIX 6.5.18 release or higher.

- RedHat Linux WS 2.1 or 3.0 running the Gnome desktop environment.

Workstation requirements

The patches required for SGI workstations are included on the QUANTA 2006 CD-ROM.

RAM and swap space requirements

We recommend that each workstation hosting QUANTA be configured with a minimum of 512 MB of memory and 1GB of swap space.

To run certain memory-intensive modules such as displaying a model in stereo view or calculating energy minimizations on large molecules, you may need additional swap space, or more RAM, or both.

Screen resolution requirements

We recomment a minimum screen resolution of 1280 x 1024.

Disk space requirements

The files installed from the distribution medium for QUANTA require the following amounts of disk space:

IRIX: 270MB

Linux: 385MB

An additional 480MB is required for database.dat (on a separate CD).

Root password requirement

In order to install this software, you must have the root password for the workstations that will host QUANTA and for your license servers. Your alternative is to have someone who knows the root passwords assist you with the installation. The root password is required to accomplish the following tasks:

- Creating the accelrys login account
- Installing the license management files into the /etc directory
- Modifying the system start-up files to include license manager information
- Mounting the distribution CD-ROM disk, if applicable

Where to install

The software is loaded into a subdirectory called Quanta_2006 in the home directory of a UNIX login account named accelrys.

2. Standard Installation

For a discussion of the choice between the standard and manual installation procedures, see Before you Install (page 3).

Sequence of events

The standard installation of this software product follows this sequence of events:

1. Create a directory to contain the product
2. Load the product's files from the release medium to the installation directory
3. Run the install script

After installing this software, perform the post-installation instructions described in After Installation (page 25).

Standard installation step by step

The following sections describe each step in the standard installation procedure.

Load the distribution medium

What you will need

Your QUANTA 2006 CD-ROM disc.

Preparing for Extraction

If you do not already have an accelrys user account please see Creating UNIX User Accounts (page 31).

Loading from CD-ROM

Accelrys products are shipped on CD-ROM in ISO 9660 with RockRidge format. The following instructions explain how to extract the software from the distribution CD.

Overview

From the UNIX shell command line, follow these steps:

- Mount the CD-ROM disk on a directory named /cdrom (or /CDROM for SGI)
- Change to the /cdrom directory
- Run the script INSTALL.EXE on the CD-ROM disk

Root password requirement

In order to mount the CD-ROM disk onto a file system, you must know the root password for the workstation to which your CD-ROM drive is connected. Your alternative is to have someone who knows the root password assist you with the installation.

Certain workstations from Silicon Graphics, Inc. do not have this requirement, as discussed in the next section.

Mounting the CD-ROM disk

The traditional directory for mounting CD-ROM disks on UNIXÆ workstations is /cdrom. If you use another directory, substitute that directory name in the instructions that follow.

Each workstation vendor uses a variation of the mount command to mount CD-ROM disks. Insert the CD-ROM disk in the CD-ROM drive (using a caddy if your CD-ROM drive requires it) and issue the mount command for your workstation.

Log in as root or another superuser account and open a command prompt session. Select the appropriate mount command from these options:

On Silicon GraphicsÆ workstations running IRIX 6.2 or later:

No mount command is necessary. Simply insert the CD-ROM disk into the CD-ROM drive. A moment later, a mount daemon automatically mounts the disk onto a directory named /CDROM. In this case, use the uppercase directory name /CDROM in the following instructions.

Running INSTALL.EXE

Follow these steps to extract the product files from the mounted CD-ROM disk:

Change to the directory on which you mounted the CD-ROM disk. For example:

```
> cd /cdrom
```

Get a directory listing and look for the name INSTALL.EXE.

```
> ls
```

On most systems, the filenames in the listing are shown in uppercase letters, but on some systems the filenames are converted to lowercase letters.

Run the INSTALL.EXE script, using the uppercase or lowercase version of the name as determined in the previous step.

```
> ./INSTALL.EXE
```

> **Note:** We recommend you do not run INSTALL.EXE as root.

The INSTALL.EXE script displays a list of the Accelrys software products on the CD-ROM disk, then checks for the existence of an accelrys user account. If found, the script prompts for permission to use the accelrys user's home directory. If you accept (**y**), the install.exe creates a subdirectory in your home directory called Quanta_2006.

> **Note:** When installing software for multiple platforms specify a different directory name for each platform.

Your ~accelrys directory is searched for an installed License Pack* directory (~accelrys/License_Pack). If none is found then you are prompted to either install the License_Pack, or to enter the path to a previously installed License_Pack. By default the License Pack is installed in the ~accelrys directory, although you can specify an alternative directory. If you already have a License Pack installed, that version is verified to make sure it is the same or newer than the version shipped with this release, and is updated if necessary.

The product list re-displays. Enter the Product_ID in the first column of the list that corresponds to the product you wish to install. Enter one Product_ID only, exactly as shown in the list.

If you told the INSTALL.EXE script in step 4 not to use the accelrys home directory, the script prompts for the path name of an alternative directory in which to extract the product's files. Enter the full path name of the alternative installation directory. The script creates a product subdirectory in the directory you specify.

When the installation directory is determined, the INSTALL.EXE script extracts the files for the product you specified. This may take as much as several hours, depending on product size, machine speed, and network traffic.

When all files are extracted, the INSTALL.EXE script re-displays the product list. If you have another Accelrys product to install, enter its Product_ID as shown in the first column of the product list. If not, type exit.

This completes the file extraction stage of the installation.

Run the install script

What you will need

You will need a valid license file named accelryslicense.dat. If a new license was emailed to you, be sure to have that license saved to a file to install during installation. If you are not a new customer, you may also be able to extract a new license during installation.

Running the script

Run install as follows:

```
> cd ~accelrys/Quanta_2006/install

> ./install
```

Specifying the start-up script path name

In the next step, the install script displays the full path name of the directory in which you installed the software. This path name will be written into the program's start-up script, so be sure it is correct. If your network uses automounted NFS drives, you may want to delete the initial /tmp_mnt portion of the path name, or if the path is not the full network path then you will want to modify it to be sure all users can access the files.

Setting the License Pack path

The install script displays the default path for the License Pack to be used with this Accelrys release. If it is incorrect, follow the prompts to enter the correct path to the License Pack.

File Configuration

Next, a list of files is displayed. These files are automatically configured with the location of this installation and the License Pack, as necessary. To modify this configuration later you may execute the config_files script at any time.

Installing the license manager

Next, the install script prompts:

```
Do you want to install the License Manager on
this machine? <y/n>
```

Respond **n** in these cases:

- Your license server will not be the same as your QUANTA host
- You already set up the license manager

If you respond **n,** the script ends. You are reminded to re-run the install script, if necessary, on the machine that will act as your license server.

Respond **y** if your QUANTA host will also act as your license server. In this case, the script looks for a license named accelryslicense.dat in the License Pack. Then:

- If the accelryslicense.dat file is found in the License Pack, the script prompts for whether you wish to replace it. If you answer **n,** the script continues to “Enabling License Manager,” below. If you answer **y,** this file is backed up to the ...License_Pack/licenses/backup directory and the license installation options appear (see below).
- If the accelryslicense.dat file is not found in the License Pack, then the license installation options appear:

```
You have the following options:
1. Extract license for your machine.
2. Extract license for another machine.
3. Extract all company licenses.
4. Install emailed or current license.
5. Continue without License Installation.
```

Options 1, 2, and 3 allow you to extract a license from licenses shipped with this

Option 1 searches for a license for the machine you are currently using.

Option 2 searches for a license for another machine, prompting you to enter a system ident.

Option 3 extracts all the licenses found for your company based on the system ident.

Option 4 allows you to enter the path to a file containing a license which was emailed.

Option 5 skips the license installation process and continues with the software installation.

Enabling the license manager

If you decide to use a previously installed license, you are prompted to start the license manager for the already installed license. If you know the daemon is already running for this license, then you can answer no to the prompts. However, if you would like to start or restart the license daemons, then answer the questions accordingly.

Once a license is extracted or installed, you are prompted to enable the license manager on the machine on which you are running the install program. If you answer yes to these prompts and have root permissions, the license daemons are set up to automatically restart at boot time as well as brought up to use with this new installation.

> **Note:** If no licenses are shipped with this release, then options 1, 2, and 3 do not appear.

Extracting/installing a license after software installation

If you choose not to install a license during the installation then you should execute the following commands, from the install directory, to do so:

```
> source ~accelrys/License_Pack/accelrys_lic_cshrc

> get_license

> reset_lic_env

> lmup (floating/token licenses only)

> license_verifier
```

Verify the license installation

Once the QUANTA files are installed, and the license manager daemon is running, you can verify the license installation by performing the following commands:

```
> source ~accelrys/License_Pack/accelrys_lic_cshrc

> license_verifier

> lmstat -a
```

(if using a token or floating license)

To test the installation and set up and configure user accounts, turn now to After Installation (page 25).

Using the Accelrys License Pack for license administration

An Accelrys License Pack is required for this Accelrys Release. A License Pack is a centralized location for all license management tools as well as the license file to support multiple Accelrys releases. The Accelrys License Pack tools and files are contained in the directory License_Pack.

To have automatic access to the License Pack tools (e.g., license_verifier, lmup -b, lmstat, etc.), enter:

```
> source <path to License_Pack>/accelrys_lic_cshrc
```

We recommend that your license administrator either place the above line in their .cshrc file, or create an alias:

```
> alias set_accelrys_lic `source \
  <path to License_Pack>/accelrys_lic_cshrc'
```

to set the license environment automatically or as needed.

Please refer to the separate *Accelrys License Guide* for details on how to manage your Accelrys license and make sure all of your Accelrys releases use the same License Pack.

Installing the SGI Dial Box

Connecting the hardware

To physically connect the dial box to your hardware, plug the dial box into an open serial port and connect the AC adapter to a power source.

> **Note:** For more information, consult the SGI dialbox installation guide:
>
> http://techpubs.sgi.com/library/tpl/cgi-bin/download.cgi?

Installing on Irix

1. To install the SGI dial box on an SGI machine, first install the eoe.sw.optinput package, available on the SGI installation CD.
2. Next, run

   ```
   > sudo /usr/sysadm/bin/runcatalog \
   /usr/sysadm/catalogdf/SaSerialDeviceCatalog.cdf
   ```

   and choose **Add Other...**.
3. In the dialog box that appears, choose **Next**, then **Input Device**, then choose the serial port you connected the dial box to. From the list of device names choose "**Dials & Buttons**", then click **OK**.

The dial box is now installed.

See Preparing the dial box for use in Quanta below.

Installing on Linux

1. To install the SGI dial box on a Linux machine, first download the XFree86 (or X.org) source code appropriate for your version of X1 (e.g., if you have WS3.0, you need XFree86 4.3.0).
2. Unzip and untar the source code in an empty directory, e.g.:

   /X11Source
3. Download the dialbox driver available here:

   http://www.geocities.com/joekrahn/
4. Run:

```
> tar xvfz dialbox.tgz
```

then:

```
> cd dialbox
```

5. Edit the makefile you find there. You should see line like "TOP = xc-4.0.1" somewhere in the file. Edit this line to read "TOP = /X11Source", where /X11Source is the path to the directory where you put the X11 source code.
6. Open the file dialbox.c in a text editor. Change the string "dials+buttons" to "dial+buttons".
7. Run make in the dialbox directory.
8. After make has successfully completed, copy the file dialbox_drv.o to your xinput directory:

```
> cp dialbox_drv.o /usr/X11R6/lib/modules/input
```

9. Add the following to your /etc/XF86Config or /etc/xorg.conf file:

```
Section "InputDevice"
    Identifier "Dialbox0"
    Driver "dialbox"
    Option "Device" "/dev/ttyS1"
    Option "EnableButtons" "off"
EndSection
```

In the 'Option "Device" "/dev/ttyS1"' line above, you should replace /dev/ttyS1 with the appropriate serial device, which is probably either /dev/ttyS0 or /dev/ttyS1, for the first or second serial ports, respectively.

10. In the same file, make sure you add the dialbox as an input device in the ServerLayout section:

```
Section "ServerLayout"
    Identifier "XFree86 Configured"
    Screen  0 "Screen0" 0 0
    InputDevice "Dialbox0"    # <-- Dialbox entry
    InputDevice "Mouse0" "CorePointer"
    InputDevice "Keyboard0" "CoreKeyboard"
EndSection
```

Note that the only line you need to add in the ServerLayout section is the 'InputDevice "Dialbox0"' line.

11. Now restart your X-server (logging off and then on should do it), and the dial box should be installed successfully.

See Preparing the dial box for use in Quanta below.

Preparing the dial box for use in Quanta

Now that you've installed the dial box, Quanta still needs to be told that you want to use it.

1. In your Quanta installation directory:

   ```
   >  cd library
   ```

2. In the file device.dat remove the # on the line"#DIAL".
3. Start Quanta. You are now ready to use the dial box with Quanta.

> **Note:** If you don't want to always enable dial box support, you can copy the device.dat file to the directory you start Quanta in and either add the '#' back to disable dial box support or remove it again to add dial box support.

3. Manual Installation

This chapter is a description of the manual installation procedure for experienced UNIX system administrators who prefer to edit start-up files directly rather than rely on installation scripts.

Sequence of events

The manual installation of QUANTA follows this sequence of events:

1. Create the accelrys user account
2. Create the directory ~accelrys/product_name
3. Log in as the user accelrys
4. Load the release medium into the installation directory
5. Configure certain site-specific files
6. Modify the hosts.equiv file.
7. Extract a license file, if available
8. Install and enable the license manager

Manual installation step by step

The following sections describe each step in the manual installation procedure.

Create an accelrys user account

Step 1. Create a UNIX user group named accelrys:

```
accelrys:*:800:
```

Step 2. Create a UNIX user account named accelrys:

```
accelrys::800:800:Accelrys Products Owner:/home/accelrys:/
bin/csh
```

Step 3. Give the accelrys account a password.

Discussion

In order to maintain a reasonable level of organization on your system, we recommend that you install all Accelrys products into the home directory of a user named accelrys. This account will only be used to hold and install products, and not for day-to-day use of a product.

If you prefer to use a name other than accelrys for this holding account, you will not have any problems. Simply substitute your account name for accelrys when reading this book.

As is true with all user accounts, it is best to put the accelrys home directory on a file system that will not be overwritten during operating system upgrades (that is, not directly on /usr).

Place the accelrys home directory on a file system with sufficient space to hold all your Accelrys products. Of course, if you run out of room on the file system that contains the accelrys home directory, you can always load a new product on another file system, and use a symbolic link to make it appear as though that product is loaded in ~accelrys.

The accelrys user must exist on all machines from which you plan to run the program. If you're not using Network Information Services (formerly known as Yellow Pages), you must create an accelrys account on each machine that will host an accelrys product.

The accelrys account must have a password to use any of the installation scripts.

Create an installation directory

Step 4. The script which unloads the software creates the subdirectory named quanta2006 in the home directory of the accelrys user. If you wish to install the software elsewhere, create that directory now.

Discussion

Using a separate directory for each product release enables you to install other Accelrys products, including future releases of this product, without disturbing the present release.

If your site supports different platforms, you should create a directory for each platform version of the software you wish to install. (See Hardware and operating system requirements (page 3)).

Log in as accelrys

Step 5. Log in (or su - accelrys) as accelrys.

Discussion

This ensures that the files loaded from the media are owned by accelrys.

Load the distribution medium

Step 6. Mount the CD-ROM disc on a directory named /cdrom, and change to this directory.

Step 7. Run INSTALL.EXE from the CD-ROM disc.

Discussion

If you are installing from CD-ROM, turn to Load the distribution medium (page 19).

Configure site-specific files

Step 8. Identify the site-specific files that must be edited. These files are listed in the product.config file.

Make a backup copy of each, then make the required edits.

Discussion

You must modify all site-specific files after the QUANTA media is loaded. The following is an example of the modifications needed for this script:

```
~accelrys/quanta2006/.setquanta
```

Search for the string %AccelrysInstallRoot% and substitute the fully qualified absolute path name of the installation directory. For example, if the home directory of the accelrys account is /home/accelrys, the lines of the script .setquanta that specify QNT_ROOT should be changed to read as follows:

```
setenv QNT_ROOT /home/accelrys/quanta2006
```

Similarly, search for the string %AccelrysLicense_Pack_Dir% and replace it with the fully qualified path name of the installation directory.

Accelrys provides a script to automate updating this file. Change to the ~accelrys/quanta2006/install directory and run the script config_files:

```
> cd ~accelrys/quanta2006/install

> ./config_files
```

Other site-specific files are supposed to be edited similarly. For the list of files to configure, see the contents of the file product.config in the install directory. If you have additional questions, contact Accelrys Scientific Support.

Modify the hosts.equiv file

Step 9. Edit your /etc/hosts.equiv or NIS-controlled hosts.equiv file, as appropriate for your network. Make sure that both localhost and the hostname of the host are recognized as trusted hosts.

Discussion

In order to start remote applications, the program needs to be able to execute a remote shell (rsh) on the machine where the remote application will run. This is done even if the application is going to run only on the local machine.

In order for this to work, the /etc/hosts.equiv file must contain two entries: one for localhost, and one for the name of the remote system.

If you are running NIS, and you either:

- Store your hosts.equiv file in an NIS-controlled master file, or
- Use netgroups in your hosts.equiv file

Then you must modify either the netgroup file, or the hosts.equiv file so that both localhost and the name of the system are recognized as trusted hosts. This will allow remote shells to be initiated without a password.

If you are not managing your hosts.equiv file through NIS, then you need to modify the product host's /etc/hosts.equiv file. You can do this manually, or you can use the update_hosts_equiv script in the install directory, as follows:

```
> cd ~accelrys/quanta2006/install

> ./update_hosts_equiv -u
```

Install a license file

Step 10. Set up the license administration environment and install a license.If you have received a license file from Accelrys by e--mail, edit and save the e-mail in a file and run get_license to install it.

If not, use the get_license script to extract a valid license file, if available. If no license is found, contact Accelrys Scientific Support to request that a license be sent via e-mail.

```
> source ~accelrys/License_Pack/accelrys_lic_cshrc

> cd ~accelrys/quanta2006/install

> get_license
```

Discussion

A **license file** is the input to the license management software used by Accelrys products. The format is too complex to edit by hand. An error in this file may cause the product to fail its license management check at run time.

For this reason it is highly recommended that you use an e-mailed copy of your license file, or use the get_license script to extract one from the media. If you must enter a license by hand (e.g., you do not have e-mail and were faxed a license) extreme care must be taken to enter the data exactly.

If using an e-mailed license file

If your license file is delivered by Internet e-mail, save the e-mail message as a file. Be sure to remove all e-mail header and trailer information from the file. The first line of your accelryslicense.dat file should begin:

```
SERVER ... or INCREMENT ...
```

The last line of your file should begin:

```
#L_INFO...
```

Make sure no extra carriage returns or spaces were added during transmission. All lines should begin with #, INCREMENT, SERVER, or DAEMON. If the character ^M appears at the end of the lines, you can use the following command to remove them:

```
> tr -d '\015' <license file> license_file.fixed
```

Use caution when editing your license file, as discussed in detail in the separate Accelrys License Guide.

The license_verifier program tells you if there are any lines with problems. You are instructed to run this when you test the installation. For more complete details on license installation refer to the Accelrys License Guide.

Install and enable the license manager (floating/token licenses only)

Step 11. Create links for the license management daemons (accelrysd and lmgrd) and the license file (accelryslicense.dat) from the directory to the /etc directory of the license server.

Step 12. Edit the license server's start-up files to launch the license daemons at system boot time.

Step 13. Remove old license daemons and startup files from the /etc directory.

Step 14. Either reboot the license server or start the license management daemons manually.

Discussion

Accelrys provides the script lmup -b to automate these steps. This script creates the necessary links to the /etc directory, edits the startup files, then starts the license management daemons. Root access is required to run this script with the -b option; you are prompted for the root password at the appropriate time.

To use the script, type these commands while logged into the host that will act as license server:

```
> source ~accelrys/License_Pack/accelrys_lic_cshrc

> lmup -b
```

If you used the lmup -b command, your installation is now complete. For final instructions, turn to Verify the license installation (page 24).

Install/enable without the script

Use the following instructions if you prefer to perform these steps without running the supplied script.

Installing and enabling the license manager involves linking certain files from the License_Pack directory to the /etc directory. If you prefer to use a directory other than /etc, please refer to the separate Accelrys License Guide.

Which license server?

The following steps should be performed while logged in to your license server.

If your license type is **node-locked** (for a single workstation), your QUANTA host does not require license daemon support. Make sure your license is in the ~accelrys/License_Pack/licenses or the $Accelrys_LIC_PACK_DIR/licenses directory and named accelryslicense.dat. You can then skip to the next section, Verify the license installation (page 24).

If your license type is float or token, your QUANTA host and your license server may be different computers. If so, be sure to copy the license files and edit the start-up scripts while logged in to the host on the SERVER line of your license. Make sure the path on the DAEMON line is ~accelrys/License_Pack/<platform>/exe/accelrysd

Link license files

For all supported host architectures using float or token licenses, the following files must be linked to the /etc directory of your license server:

```
> ln -sf ~accelrys/License_Pack/<platform>/exe/lmgrd
  \
  /etc/lmgrd

> ln -sf ~accelrys/License_Pack/licenses/accelrysli-
  cense.dat \
  /etc/accelryslicense.dat

> ln -sf \
  ~accelrys/License_Pack/logs/accelryslicense_
  <port>.log \
  /etc/accelryslicense_<port>.log
```

Edit startup files

The next steps vary for each host architecture:

For Silicon Graphics workstations, use these commands:

```
> sed -e “s@%LOCKAccelrys%@lockaccelrys_<license
  970@g; \
  s@%LICENSE%@accelryslicense.dat@g; \
  s@%LOGFILE%@accelryslicense_<port>.log@g; \
  s@%NON_ROOT_USER%@<accelrys or other user name>@g”
  \
  ~accelrys/License_Pack/bin/accelrys_lmbo

> cp /tmp/accelrys_lmboot /etc/init.d/accelrys_lmboot
```

```
> ln -sf /etc/init.d/accelrys_lmboot \
  /etc/rc2.d/S99accelrys_lmboot

> ln -sf /etc/init.d/accelrys_lmboot \
  /etc/rc0.d/K10accelrys_lmboot
```

Remove old start-up files manually or by running:

```
> ~accelrys/License_Pack/bin/rm_old_accelryslm sgi
```

Note: Due to possible security problems the license manager daemons must be run as a non-privileged (non-root) user.

Start the license manager daemon

Once the above files have been copied and edited, you can start the license manager daemon with these commands:

```
> /etc/lmgrd -c /etc/accelryslicense.dat \
  >>/etc/accelryslicense_<port>.log
```

Again, instead of performing all steps manually, we highly recommend that you run **lmup -b** as described in Install and enable the license manager (floating/token licenses only) (page 22).

Verify the license installation

Once the product files are installed, and the license manager daemon is running, you can verify the license installation by performing the following commands:

```
> source ~accelrys/License_Pack/accelrys_lic_cshrc

> lmup

> license_verifier

> lmstat -a
```

(if using a token or floating license)

To test the installation and set up and configure user accounts, turn now to After Installation (page 25). For more complete license management information refer to the separate Accelrys License Guide.

4. After Installation

This chapter shows how to set up and configure user accounts for QUANTA.

Testing the installation

To start the program, type the following line at the shell prompt:

```
> source ~accelrys/quanta2006/.setquanta
```

Now you have an alias named quanta. To run a one-time test of the installation, type the alias name as the command to run the program:

```
> quanta
```

Setting up user accounts

The .cshrc file of each user authorized to run QUANTA must source the installed .setquanta file. Edit the .cshrc file of each qualified user, adding the following line:

```
source ~accelrys/quanta97/.setquanta
```

After the next login, you can type this command to invoke the program:

```
> quanta
```

These fields must match

Install database.dat

To install database.dat in an exising QUANTA installation do the following:

1. Make sure your QUANTA environment is initialized.
2. Change to the directory containing this README:

```
> cd /path/to/database/cd
```

3. Backup your existing database.dat file:

```
> cp $HYD_LIB/database.dat $HYD_LIB/database.bak
```

4. Copy the database.dat file in this directory to your QUANTA installation directory:

```
> cp database.dat $HYD_LIB/database.dat
```

Configuring SGI to run in 24 bit TrueColor mode

SGI boxes must be configured to run in 24 bit TrueColor mode to run the X11 version of quanta.

True Color mode is an X windowing environment mode on IRIX that enables applications to make use of the 24-bit color depths available on video cards and monitors. This color depth is supported by all SGI workstations Octane and newer. Graphics intensive programs typically require True Color.

To set up:

1. Log in as root.
2. As a precaution before editing, make a backup copy of the file /var/X11/xdm/Xservers.
3. Edit /var/X11/xdm/Xservers as follows:

   Original: :0 secure /usr/bin/X11/X -bs -nobitscale -c -pseudomap 4sight -solidroot sgilightblue -cursorFG red -cursorBG white

   Change to: :0 secure /usr/bin/X11/X -bs -nobitscale -c -class TrueColor -depth 24 -solidroot sgilightblue -cursorFG red -cursorBG white

4. Run the following command (logging out does not reset the display):

   (/usr/gfx/stopgfx; /usr/gfx/startgfx)&

> **Note:** Both “stopgfx” and “startgfx” must be run *at the same time and on the same command line*. If they are not, you will not be able to re-login properly.

Stereo in a Window (SGI)

Running QUANTA in stereo in a window mode on SGI requires that you have pre-configured your X Server to support hardware stereo. This configuration is typically performed by the root user using the /usr/bin/X11/xsetmon command. xsetmon provides an interactive interface to select the video mode as the default value for future X Windows sessions. Changing video modes typically requires restarting the X Server, which is accomplished by logging out and logging back in.

When selecting a mode for QUANTA stereo, be aware that only modes ending in “s” support hardware stereo. Also note that refresh rates around 100Hz or better produce the most realistic stereo image in the application (since each eye is refreshed at 50Hz). For example, on the workstations at Accelrys we typically use the 1280x1024_96s mode, which gives a resolution of 1280x1024 pixels and a refresh rate of 96Hz.

For more information on using xsetmon and video modes please refer to the SGI IRIX system administration guides. You can also access the xsetmon and related manual pages from the SGI website:

http://techpubs.sgi.com/

To test these changes from within QUANTA, perform the following steps:

1. Enter:

   ```
   > quanta
   ```

2. Load a molecule.
3. To view molecules in stereo, select **View | Stereo | Stereo in a Window** or type **VIEW SWIN**.

Stereo in a Window (Linux)

Running QUANTA in *Stereo in a Window* mode on Linux requires that you have configured your XF86Config file set to enable the “Stereo” option. Once you have downloaded and installed the NVidia drivers, you must make changes to the file /etc/X11/XF86Config-4 as follows:

1. Make sure the “Device” section is using the “nvidia” driver.
2. Add the following line to the “Screen” section:

   ```
   Option "Stereo" "3"
   ```

Examples of these sections are below:

```
Section "Device"
            Identifier   "Device0"
            Driver       "nvidia"
            VendorName   "Device0"
            BoardName    "Device0"
     EndSection

     Section "Screen"
            Identifier   "Screen0"
            Device       "Device0"
            Monitor      "Monitor0"
            DefaultDepth    24
            Option "Stereo" "3"

            Subsection "Display"
                    Depth       24
                    Modes       "1600x1200"
            EndSubsection
     EndSection
```

To test these changes from within QUANTA, perform the following steps:

1. Enter:

   ```
   > quanta
   ```

2. Load a molecule.
3. To view molecules in stereo, select **View | Stereo | Stereo in a Window** or type **VIEW SWIN**.

A. License Administration

The contents of the license administration appendix have been expanded and moved to the separate Accelrys License Guide available at the following URL:

http://www.accelrys.com/support/license_info.html

B. Creating UNIX User Accounts

A system user named accelrys must exist in order to install Accelrys software products. This user exists solely for the purpose of installing, testing, and owning the product distribution. This account is not intended for day-to-day use of the product.

This appendix is intended to be a reminder for Accelrys users who are not full-time system administrators. The reader should have a basic knowledge of the UNIX file system and the use of a text editor. The instructions below presume the use of the vi editor.

Modify the /etc/passwd file

Step 1. Log in as the root user on the workstation that will serve as the primary host for the Accelrys product. Change to the /etc directory and prepare to edit the file passwd:

```
> cd /etc
```

```
> vi passwd
```

The passwd file is composed of records, one record per line. Each record is divided into fields separated by colons. Inspect the file to be sure there is no line with 800 in either the third or fourth field.

Step 2. Go to the bottom of the file by typing an uppercase G. Inspect the file again and look for a line near the bottom that begins with a plus sign (+). If you find such a line, move the cursor to the line above it. If no line begins with a plus sign, move the cursor to the last line of the file.

Step 3. Open a new line by typing an uppercase O. Add the following line exactly as shown here:

```
accelrys::800:800:Accelrys Products Owner:/home/accelrys:/bin/csh
```

If you found an instance of 800 in the first step, change the corresponding 800 in this line to 801.

The above line defines the user accelrys as follows:

Table 1

Field	Field Contents	You enter
1	user name	msi
2	password	blank (will be added later)
3	user id no.	800
4	group id no.	800
5	description	MSI Products Owner
6	home directory	/home/msi (or appropriate path name)
7	initial shell	/bin/csh

The sixth field contains the full absolute path name of the accelrys account's home directory. If the target host has no /home file system, substitute the appropriate path name.

Step 4. Once you enter a properly formatted line for the accelrys account, press Esc and write the file to disk:

```
:wq!
```

The exclamation point forces the edit on this file even if it is configured to be uneditable in your environment.

Assign a name to the accelrys group

Step 1. To assign the name accelrys to group number 800, add an entry to the /etc/group file:

```
cd /etc
vi group
```

Step 2. Inspect the file to make sure that a group numbered 800 does not already exist. Now go to the bottom of the file by typing an uppercase G. If the last line begins with a plus sign

(+), move the cursor to the line above it. Open a new line by typing an uppercase O. Define the group accelrys by adding the following line:

```
accelrys:*:800:
```

Step 3. If your inspection showed an existing group 800, substitute 801 in this line. Make sure the group number in the third field of the accelrys entry in this file matches the group number in the fourth field of the accelrys entry in the passwd file:

```
accelrys:*:801:
accelrys::800:801:Accelrys Products Owner:/home/accelrys:/bin/csh
```

Step 4. Press Esc and write the file to disk: :wq!

Create the accelrys home directory

Step 1. As the root user, make sure you're running the C-Shell (/bin/csh) before you create the accelrys home directory. Type:

echo $0 If the response is No file for $0, continue to step 2. If the response is anything else, invoke a C-Shell session as follows:

```
/bin/csh
```

Step 2. Create the accelrys home directory by typing the following:

```
mkdir ~accelrys
chown accelrys ~accelrys
chgrp accelrys ~accelrys
chmod 777 ~accelrys
```

Add a password to the accelrys account

In order for all of the installation scripts to work correctly, the accelrys account must have a password. To add a password to the accelrys account, login as accelrys and use the passwd command as follows: passwd

```
passwd: changing password for user accelrys
enter new password: *******
re-enter new password: *******
```

The password must be typed the same way both times for the system to accept it. The password does not appear on the screen as you type it.

C. The applcomm.db File Format

Accelrys applications store this information in a human-readable file similar in concept to the UNIX file /etc/services, which lists network services and the ports on which they are available. This application communications database file is named applcomm.db.

Under normal circumstances, applcomm.db is edited automatically during installation of the invoking Accelrys application and does not need to be altered. This appendix documents the file's format for those cases when you need to augment the information in this file.

File contents

The applcomm.db file contains records describing machines in the network, possible communication protocols, and applications that can be run on those machines.

Three different types of records can appear in this file. The symbol in the first position of each line is a control character and must be one of the following:

- Comments

M - Records describing machines in the network

P - Records describing communication protocols

A - Records describing applications

The following points apply to record lines in general:

- Empty records (containing only spaces and/or tabs) are legal and are treated as comments
- All other records are ignored, but a warning message is displayed with the contents of the ignored record
- Fields in the records are separated by spaces and/or tabs

Records describing machines

The following points apply to record lines that describe machines on your network:

- Machines can be (but need not be) grouped in classes. There is no special meaning in the class name, with the exceptions of MVS and manual.
- One machine may belong to more than one class.
- Classes (and machines) can also be grouped. However, looping is forbidden: if class A belongs to class B, class B may not belong to class A.
- Grouping in classes helps the coding of A-records.
- If a machine is not defined in any M-records, it gets assigned the class default.

The format of an M-record is as follows:

```
M class machine1 [machine2 ...]
```

where:

class Name of the class, which can be any arbitrary name.

machine Name of a remote machine or a machine class.

Examples:

```
# SGI
M slow beauty bohr clover dirac watson
M medium bam-bam buster dino gomez ram
M fast altoid newton null
M Indigo ram buster dino null
M sgi slow medium fast Indigo

# Other machines
M rios hanz franz hogan
M hp720 avoid devoid

# all of them

M unix sgi rios hp720
```

Records describing supported network protocols

The format of a P-record is as follows:

```
P protocol machine1 [machine2 ...]
```

where:

protocol Either unix or tcp

machine Either the actual host name or a class name as defined in an M-record

If a machine is not defined in any P-records, UNIX protocol is accepted for a local UNIX machine, and tcp otherwise.

Examples:

```
P unix unix
P tcp unix eagle.tc.cornell.edu rain.cray.com
```

Records describing supported applications

The format of an A-record is as follows:

```
A machine application executable [argument [...]]
A class application executable [argument [...]]
```

where:

machine Actual host name on which application is available

class A machine class, defined by an M-record

application The application name (charmm, xplor, and so on)

executable The command that should be executed on the machine to run the application (If this

command does not exist in the user's default path, the full path name must be given in the A-record.)

argument Any argument that must be passed to the application

An A-record is necessary for every application that you want to start by using the Accelrys remote job module.

Examples:

```
A remote_unix rjrd /home/accelrys/quanta/exec/rjrd
A remote_unix xplor /home/accelrys/xplor/xplor.bat
```

Example applcomm.db file entries

The following applcomm.db extract contains example entries for quantum applications.

```
# These lines specify the locations of the ADF
# files. You may need to alter the specifications
# if you want to run ADF on a machine on which you do
```

```
# not have Cerius2 licensed. A SGI adf c2_install_dir/exec/adf.exe
A SGI ADFBIN c2_install_dir/adf/bin
A SGI ADFUTILITIES c2_install_dir/adf/bin
A SGI ADFRESOURCES c2_install_dir/Cerius2-Resources/ADF/atomicdata
# The following line specifies the location of the main
# Gaussian 92 directories. Replace the path name with that
# for your own installation. If you don't have Gaussian
# 92, omit this line.
A SGI g92root /usr/mydir/gaussian92
# The following line specifies the location of the main
# Gaussian 94 directories. Replace the path name with that
# for your own installation. If you don't have Gaussian
# 94, omit this line.
A SGI g94root /usr/mydir/gaussian94
# The following lines specify an alternative location for the
# Gaussian 92 and Gaussian 94 scratch directories. If this
# line is omitted, the current working directory is used.
A SGI g92scratch /usr/disk2/gaussian.scratch
A SGI g94scratch /usr/disk2/gaussian.scratch
# The following two lines are standard. Only change them
# if you have a non-standard installation, or if you
# want to run mopac on a machine on which you do not
# have Cerius2 installed.
A SGI mopacdir c2_install_dir/mopac
A SGI mopac6exe c2_install_dir/mopac/mopac6.exe
# The following line specifies the location of the MOPAC7
# executable. If you don't have MOPAC7, omit this line.
A SGI mopac7exe /usr/mydir/mopac7/mopac7_sgrw/mopac.exe
# The following line specifies the location of the MOPAC93
# executable. Replace the path name with that of your own
# installation. If you don't have MOPAC93, omit this line.
A SGI mopac93exe /usr/mydir/mopac93/m93_src/mopac93.exe
# The following line specifies the location of the
# DMol3 executable. Only change it if you have a
# non-standard installation, or if you want to run DMol3
# on a machine on which you do not have Cerius2 installed.
A SGI dmol3exe c2_install_dir/exec/dmol3
```

D. Configuring an IBM T42p ThinkPad for Red Hat Enterprise Linux

This document details how to install Red Hat Enterprise Linux on a bare IBM T42p ThinkPad for using Accelrys' Linux-based products. Specifically, these instructions are customized for RHEL 3.0 WS Update 3 with version 8.8.25 of the ATI unified video drivers.

1. Install the OS

Install RHEL WS 3.0 Update 3 (U3).

2. Video Configuration

This machine has an ATI MOBILITY FIRE GL T2 graphics card. Use the proprietary closed-source driver from ATI to provide accelerated 3D OpenGL support. The driver can downloaded from ATI here:

http://www.ati.com/

You should use version 8.8.25 for XFree86 4.3.

Notes on installing the ATI driver

The ATI website provides a driver in rpm format. It is documented on their site that this RPM conflicts with the Mesa libraries that are required for certain Accelrys products. According to ATI the procedure is to force installation of their driver.

```
> rpm -Uh --force fglrx_4_3_0-8.8.25-1
```

This has the effect of replacing the GL shared objects that came from Mesa with the ones from the ATI driver. Check this by using the verify options for both packages:

```
> rpm -V fglrx_4_3_0-8.8.25-1

> rpm -V XFree86-Mesa-libGL-4.3.0-68.EL
```

Only the XFree86-Mesa package should give conflicts for the following files and links:

```
....L...   /usr/X11R6/lib/libGL.so.1
S.5...GT   /usr/X11R6/lib/libGL.so.1.2
....L...   /usr/lib/libGL.so.1|
```

After forcing the driver installation, the kernel module then needs to be built and installed:

```
> cd /lib/modules/fglrx/build_mod/

> sh make.sh

> cd /lib/modules/fglrx/

> sh make_install.sh
```

This procedure may give errors about not being GPL'd software resulting in a tainted kernel. The ATI website says this message may be ignored.

Now configure the graphics:

- Run the fglrxconfig tool. Use the defaults.
- Run the Red Hat video configuration tool, redhat-config-xfree86. This tool allows the monitor and video hardware lists in the GUI to be specified, but also preserves the unique options generated by the fglrxconfig tool.
- The redhat-config-xfree86 program will automatically rename the file as “XF86Config” upon exit, avoiding confusion which can occur if the deprecated XF86Config-4 name is in use.

This should generate a “XF86Config” in /etc/X11.

Now reboot the machine. Check that ATI kernel module is present using the 'lsmod' command - it should list fglrx:

```
> lsmod | grep fglrx

fglrx                  221160   8
```

Then run an OpenGL demo to check the frame rate and confirm that the graphics are hardware accelerated. Glxgears should exceed 1000 fps.

```
> glxgears # or,

> stars
```

The latter is downloadable from:

http://www.cr0.net:8040/code/opengl/demos.tgz

Modem

T42p has a new Conexant-based modem. While the “shareware” driver is available from Linuxant, this restricts download to 14.4k. Instead use the full-functioning drivers available from IBM.

USB Mouse

To enable an external USB mouse add the following lines to /etc/x11/XF86Config and then reboot the machine:

```
# If the normal CorePointer mouse is not a USB mouse then
# this input device can be used in AlwaysCore mode to let you
# also use USB mice at the same time.
Identifier  "DevInputMice"
Driver      “mouse”
Option    “Protocol” “IMPS/2”
Option    “Device” “/dev/input/mice”
Option    “ZAxisMapping” “4 5"
Option    “Emulate3Buttons” “no”
EndSection
```

This document contains no index.