Linux Desktops Documentation

Release RHEL7

University of Southampton

Aug 17, 2018

Basics

Welcome to the documentation for Linux Desktops at the University of Southampton

CHAPTER 1

Desktop Manager

You can manage your desktop using the Desktop Manager tool. Log in to your desktop computer, open a web browser and go to the following location:

https://deskctl

You can also open the Desktop Manager tool within GNOME by press the Start button and searching for “Desktop Manager” and then selecting the resulting entry for the tool.

Desktop manager allows you to:

- Install software, including University provided software
- Manage permissions (change who can do what)
- Check the status of backups
- Start a backup on demand
- Check the software update status
- Check the health of the system
- View the system hardware information
- Open this documentation

CHAPTER 2

Installing software

2.1 Desktop Manager

The recommended method for installing software is via the *Desktop Manager* tool. This tool contains specialist software, packages created by iSolutions, and all software specifically requested by members of the university. If a package is missing from it, and you think it should be listed, let us know!

2.2 GNOME Software

You can also use the GNOME Software tool to install software. It only includes graphical applications (GUI apps) and does not include specialist software or packages created by iSolutions.

It does however include most of the default GUI software in Red Hat Enterprise Linux so if you're looking for a standard GUI application then GNOME Software will probably let you install it.

To start GNOME Software press the Start button and search for "Application Installer".

2.3 yum

If you're not afraid of the command line then the easiest and fastest way to install software is to use `yum`. You can search for software like this:

```
sudo yum search <name>
```

You can then install a package once you've found it like this:

```
sudo yum install <package-name>
```

Or remove a package:

```
sudo yum remove <package-name>
```

CHAPTER 3

Backups

Your home directory is backed up automatically at least once a day.

3.1 When are backups taken?

Your workstation will attempt to back up all the data in `/home` between 11pm and 12am. If your computer is switched off at this time do not worry, the next time you start your computer a backup will be attempted then instead.

3.2 Do I need to keep my computer on overnight?

You do not need to leave your computer on overnight. If you prefer to keep your computer turned off then backups will still take place. Whenever your computer starts up it determines if a backup should be taken and then initiates a backup if required.

3.3 How long are backups kept for?

Backups of each workstation are kept for 30 days after the backup was taken.

If your machine is not switched on, or otherwise unavailable, for 30 days, then all backup data will be deleted. To ensure you always have a copy of data in case of hardware failure please ensure your computer takes at least one backup a month.

3.4 How can I check the backups are working?

You can use *Desktop Manager* to check the status of the last backup attempt.

You can also run the following command in a terminal:

```
sudo drone backup status
```

3.5 Can I trigger a backup?

Yes you can start a backup whenever you need to. This allows you, for example, to take a backup before turning your computer off before leaving the office. You can start a backup using *Desktop Manager* or if you prefer you can run the following command in a terminal:

```
sudo drone backup now
```

3.6 Can I use my PC whilst a backup is underway?

Yes. The backup system takes a snapshot of the data when the process begins and backs up the data in the snapshot. You can thus carry on using your computer without affecting the backup (or the backup affecting your data). The backup system uses LVM thin snapshots to accomplish this.

3.7 Do backups work when outside the University network?

For the backups to work you must connect to the University network via one of these methods:

- Connect to the university network via an Ethernet cable
- Connect to the `eduroam` wireless network
- Connect to the university virtual private network (VPN) service

3.8 Can backups be disabled?

In very rare circumstances iSolutions will disable backups on a workstation.

To do this, you need to be a member of iSolutions staff with root access, and you run the following command to do so:

```
sudo drone backup disable
```

Backups can be then enabled again at a later date with:

```
sudo drone backup enable
```

CHAPTER 4

Local storage

4.1 Your home directory

- Location: `/home/$username/`
- Backed up: `Yes`

Your home directory is stored on the computer's local drive. This data is backed up every day - see *Backups* for details. You are not limited by a quota but the `/home` partition/drive is only 50GB in size. If you expect your computer to be used by multiple people please be considerate and don't use *all* the space on the partition.

You can check the usage of the drive in *Desktop Manager*

4.2 Local scratch space

- Location: `/local/scratch/$username/`
- Backed up: `No`

If you need space for large amounts of data you should store this within your local scratch space. This space is however not backed up, so don't store anything important there!

The scratch space is stored within the `/local` partition, thus this is only limited by the size of the drive within your computer.

You can check the usage of the drive in *Desktop Manager*

4.3 Other locations

Some computers have multiple drives installed, in which case an iSolutions technician will have set up the second drive at `/data`. Directories are not automatically created within this location. Any data stored there is not backed up.

CHAPTER 5

Network storage

5.1 Available locations

There are several storage systems available to connect to on the University network:

5.1.1 Personal Filestore (via SSH)

- Location: `sftp://ssh.soton.ac.uk/home/$username/`
- Protocol: `SSH/SFTP`
- Linux friendly semantics: `Yes`

This is your central university storage or 'filestore'. Data stored here is backed up and available on Linux, Windows and Mac OS X computers. You can also access data stored here via Filestore Web Access.

5.1.2 Personal Filestore (via SMB)

- Location: `sftp://ssh.soton.ac.uk/home/$username/`
- Protocol: `SMB1`, `SMB2`
- Linux friendly semantics: `No`

You can also access your personal filestore via the SMB protocol (the Windows file sharing protocol). If you connect via this method then you will not be able to set or view file/directory permissions, create symbolic links or use any other POSIX (Linux/UNIX) features. Due to this it is *strongly* recommended that you utilise SSH instead.

5.1.3 Linux Shared Filestore

- Location: `sftp://ssh.soton.ac.uk/research/$groupname/`
- Protocol: `SSH/SFTP`

- Linux friendly semantics: `Yes`

Many research groups and departments have access to shared storage locations specifically designed for use from Linux systems. These are available at the above location. Data stored here is backed up. You can also access data stored here via Filestore Web Access.

5.1.4 Other Shared Filestore

- Location: `smb://filestore.soton.ac.uk/$sharename/`
- Protocol: `SMB1`, `SMB2`
- Linux friendly semantics: `No`

Many other shared locations exist, such as the “J: drive” shared storage locations. These are available at the above location. Data stored here is backed up. You can also access data stored here via Filestore Web Access.

These locations are unfortunately designed for use by Windows users. You will not be able to set or view file/directory permissions, create symbolic links or use any other POSIX (Linux/UNIX) features.

5.2 How to connect

There are various methods of connecting to network storage:

5.2.1 via the file browser

If you’re using GNOME (the default), XFCE, MATE or KDE then you can simply open the file browser and enter the location you want to connect to by pressing `Ctrl+L` or clicking `Connect to server` in the menu. You will be prompted for a username and password as necessary.

We strongly recommend you use this mechanism to connect to network storage. You can also access the connected storage from other applications and the command line. Once connected they are available via the normal file system here:

```
/run/user/$uid/gvfs/
```

5.2.2 via FUSE (SSH only)

If you prefer to connect to networked storage on the command line only, you can do so using the `sshfs` command. We strongly recommend you use the above mechanism (the file browser) instead since that can also be accessed from the command line.

If you do want to use `sshfs` directly then run the command like so:

```
sshfs [user@]host:[dir] mountpoint
```

For example, here is how to connect to your personal filestore as `testuser`:

```
mkdir ~/personalfs
sshfs testuser@ssh.soton.ac.uk:/home/testuser/ ~/personalfs
```

You can then later disconnect with:

```
fusermount -u ~/personalfs
```

5.2.3 via the `mount` command

You can also instruct the kernel to mount network storage if you desire. This can however be quite complicated and this documentation only covers the basics.

You can use the `mount` command via `sudo` if you are in the `sys` group (see *Permissions* for more information). You can thus use the command like so:

```
sudo mount <options>
```

Here is an example of how to mount personal filestore via the `cifs` driver with the example username `testuser`:

```
mkdir ~/personalfs
sudo mount -t cifs -o username=testuser,password=<password>,domain=soton.ac.uk //
↪filestore.soton.ac.uk/users/testuser/ /home/testuser/personalfs/
```

CHAPTER 6

Printing

The university uses a 'follow me' printing service where you can submit a print job from your desktop and then print from any multi-function printer (MFD) on the university network.

There are two default printer queues set up for this on your Linux desktop which you can use 'out of the box'. The queues are called `mono` and `colour`. The first time you print to either of them you will be prompted to enter your university username and password. Sadly owing to limitations in CUPS (the Linux printing system) we cannot automatically authenticate you. Instead you can opt to save your username and password, and the password is stored in your GNOME keyring (where it is encrypted).

If you have administrator rights granted to you on your desktop (i.e. you are in the `sys` group), you can add and edit printers. You may want to add a new printer if you are in a lab which has a printer other than the normal University MFDs.

To add such a printer:

1. Open the GNOME Settings application (Applications -> System Tools -> Settings) and then choose Printers. Note that you may also find Print Settings, which is a separate method of adding a printer and not documented here.
2. Choose Unlock and, if prompted, enter your username and password to authenticate.
3. Next, click the plus (+) button that's underneath the list of printers and the Add a New Printer dialog will appear.
4. In the text box at the bottom of the dialog, enter: `smb://servername/`, where `servername` should be listed on the label on the printer you wish to add. `servername` will often be something like `server1.printing.soton.ac.uk`.
5. As you enter this you will be prompted to authenticate to the print server, after which, you should be given a list of printers.
6. Double-click on your printer from the list - it should match the name that is on the label on the printer, e.g. `PR_B12_R3456_P01`
7. Next, the Select Printer Driver dialog should appear. Choose `Generic` from the list on the left and then `Generic PostScript Printer` from the list on the right.
8. Press the Select button.

9. The printer is now added to the system, and you should now be able to print to it
10. Note that you can’t set a system-wide default printer here as that is managed by system policy (and if you manage to change it, it will get reverted), however you can change the default printer for your account on your desktop using the documentation below.

To change the default printer:

1. Open the Print Settings application
2. Right-click the printer you wish to make the default for you
3. Choose Set as Default from the menu
4. Choose Set as my personal default printer
5. Click OK

CHAPTER 7

E-Mail

At present, the univerity's e-mail solution is Microsoft Exchange for most staff and Office 365 for students.

7.1 Using Outlook web access

The easiest way to access your e-mail (and calendars and contacts) is to use Outlook web access:

- Staff and postgraduates: www.outlook.soton.ac.uk
- Students: www.outlook.com/soton.ac.uk

7.2 Using GNOME / Evolution

The next easiest way to access your e-mail (and contacts) is to use the e-mail client in GNOME - evolution. The fastest way to set it up is to open Settings and click `Online Accounts`.

- Click "Add an online account"
- Choose "Microsoft Exchange"
- Enter the E-Mail as yourusername@soton.ac.uk
- Enter your normal university password

Open Evolution and your e-mail account will have automatically been created.

7.3 Using other clients

If you decide to use another e-mail client you'll likely want to use IMAP and SMTP for sending and receiving e-mails. The support in Microsoft Exchange for IMAP clients is very poor however (performance is appauling and the IMAP server is not very compliant to the RFC - surprising, no?). We thus recommend either using Outlook Web Access or Evolution, but if you really do want to take the plunge, here are the details:

- IMAP server: `imap.exchange.soton.ac.uk`
- IMAP security: SSL/TLS (port 993)
- SMTP server: `smtp.soton.ac.uk`
- SMTP security: STARTTLS (port 25)

CHAPTER 8

Installation

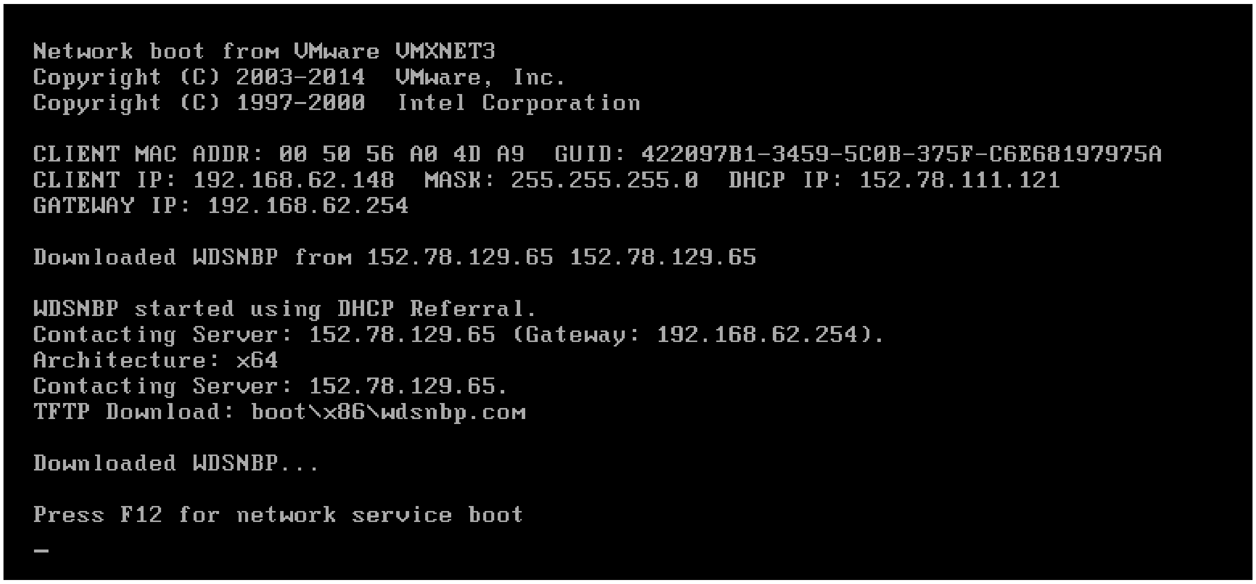
Note: To install the University Linux Desktop system you need to be a member of iSolutions staff (i.e. in the 'jfStaff' group). We are working on a way for anybody to install Linux desktops, but this is not yet available.

8.1 Before you begin

- Ensure that no USB hard drives or thumb drives are attached
- Ensure that no non-standard devices are attached by USB or otherwise
- Check for second or third hard drives. These should not be wiped, but if they contain data customers want, best practice is to disconnect them first.
- Make sure the PC is set to BIOS mode (not UEFI)
- Ensure Hybrid graphics are disabled, if offered

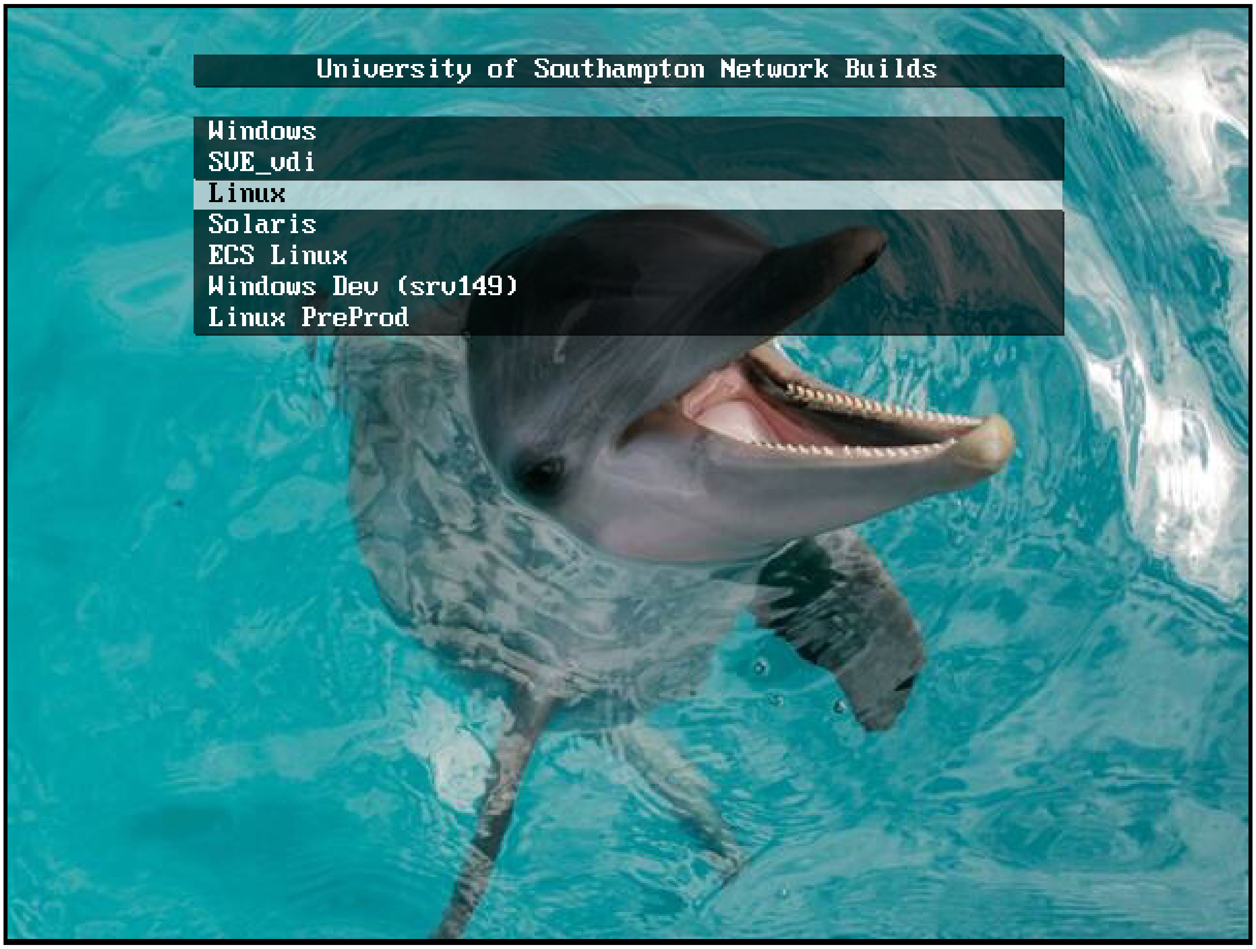
8.2 Start the installation

Turn the computer on and select network boot (PXE boot) as it starts. When prompted, press F12 to start the network installation system:

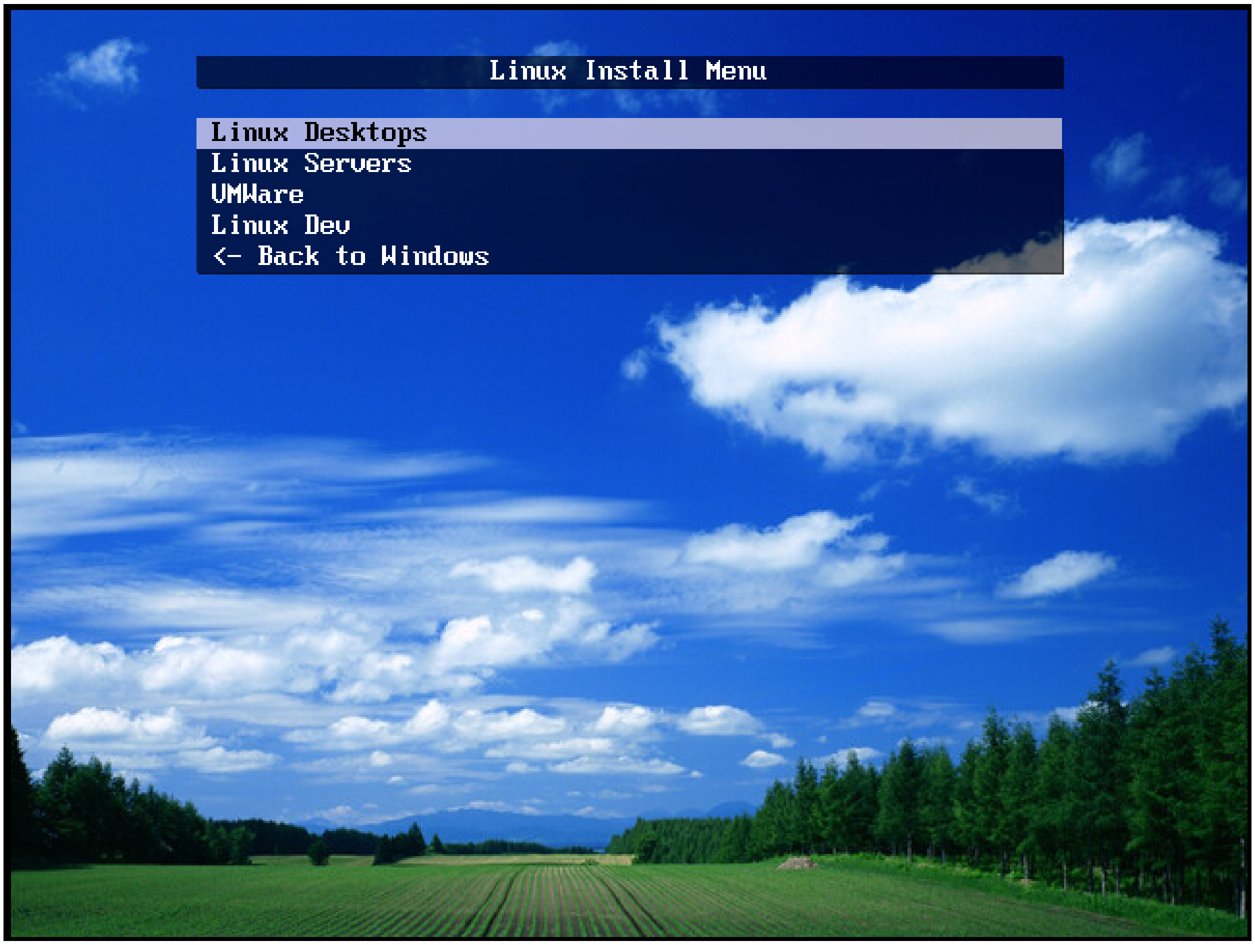


```
Network boot from VMware VMXNET3
Copyright (C) 2003-2014  VMware, Inc.
Copyright (C) 1997-2000  Intel Corporation

CLIENT MAC ADDR: 00 50 56 A0 4D A9  GUID: 422097B1-3459-5C0B-375F-C6E68197975A
CLIENT IP: 192.168.62.148  MASK: 255.255.255.0  DHCP IP: 152.78.111.121
GATEWAY IP: 192.168.62.254

Downloaded WDSNBP from 152.78.129.65 152.78.129.65

WDSNBP started using DHCP Referral.
Contacting Server: 152.78.129.65 (Gateway: 192.168.62.254).
Architecture: x64
Contacting Server: 152.78.129.65.
TFTP Download: boot\x86\wdsnbp.com

Downloaded WDSNBP...

Press F12 for network service boot
_
```

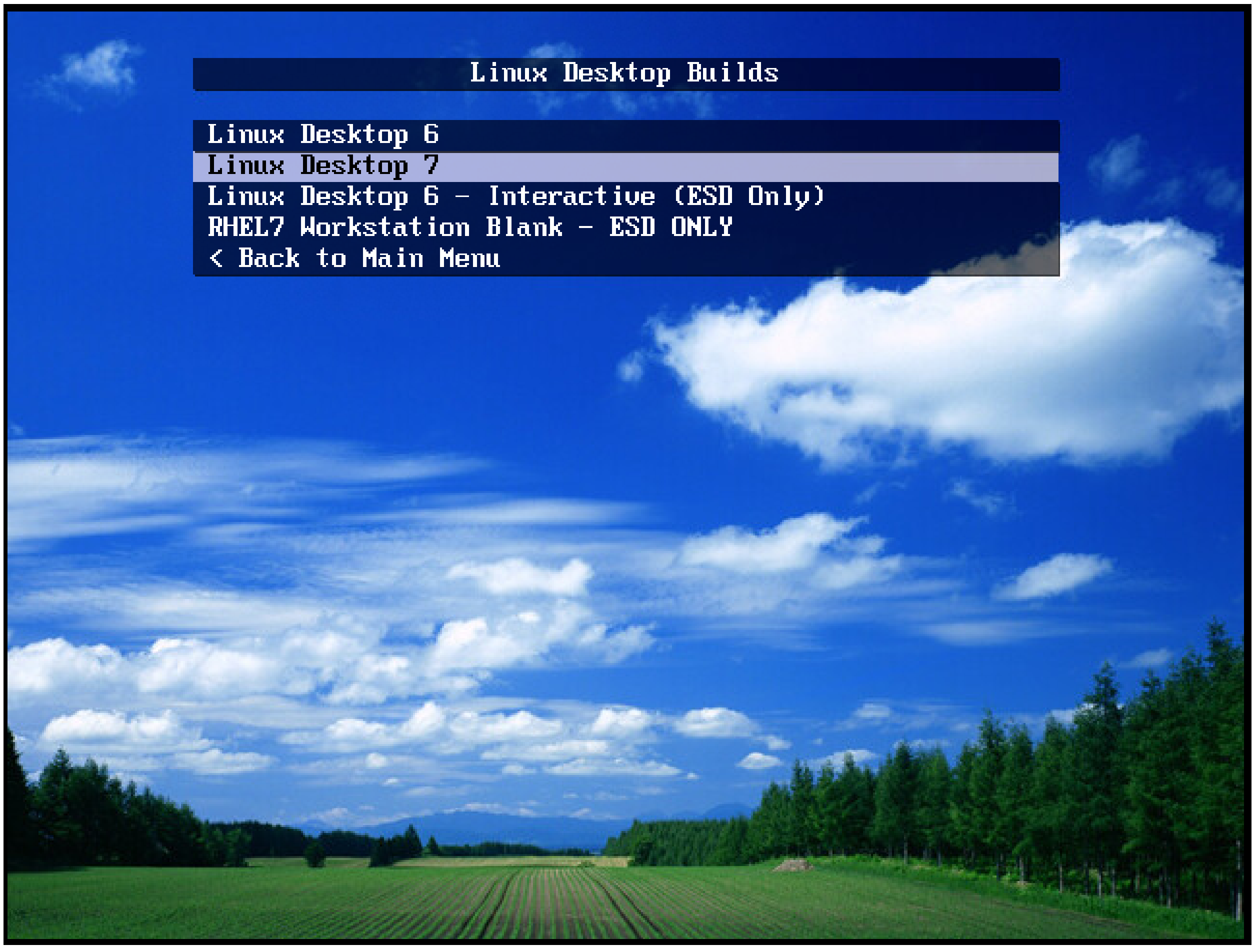
The network build menu should then appear, choose Linux:



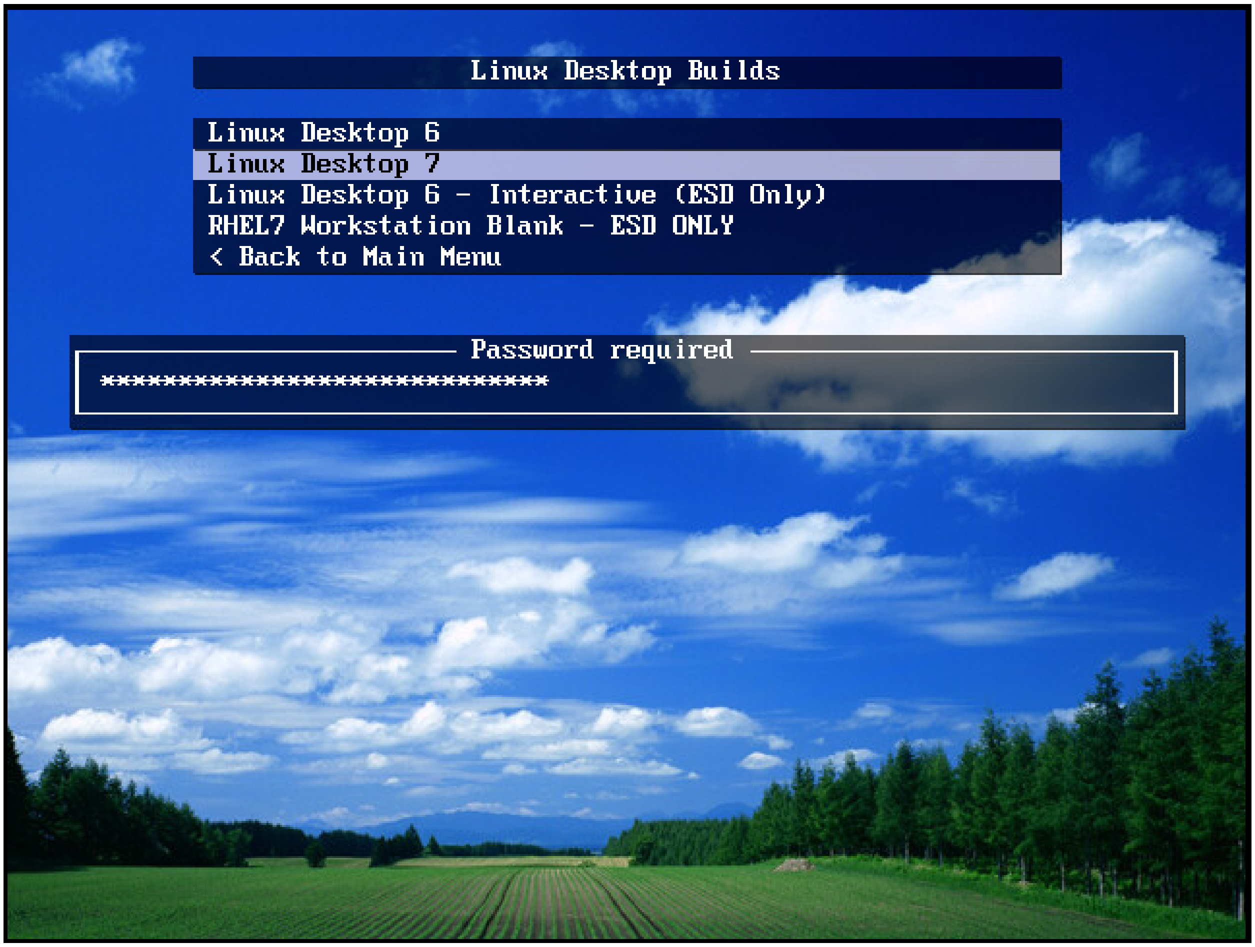
and then on the next menu choose Linux desktops:



Finally, choose Linux Desktop 7:


Linux Desktop Builds
Linux Desktop 6
Linux Desktop 7
Linux Desktop 6 - Interactive (ESD Only)
RHEL7 Workstation Blank - ESD ONLY
< Back to Main Menu

You will be prompted for the Linux build password:

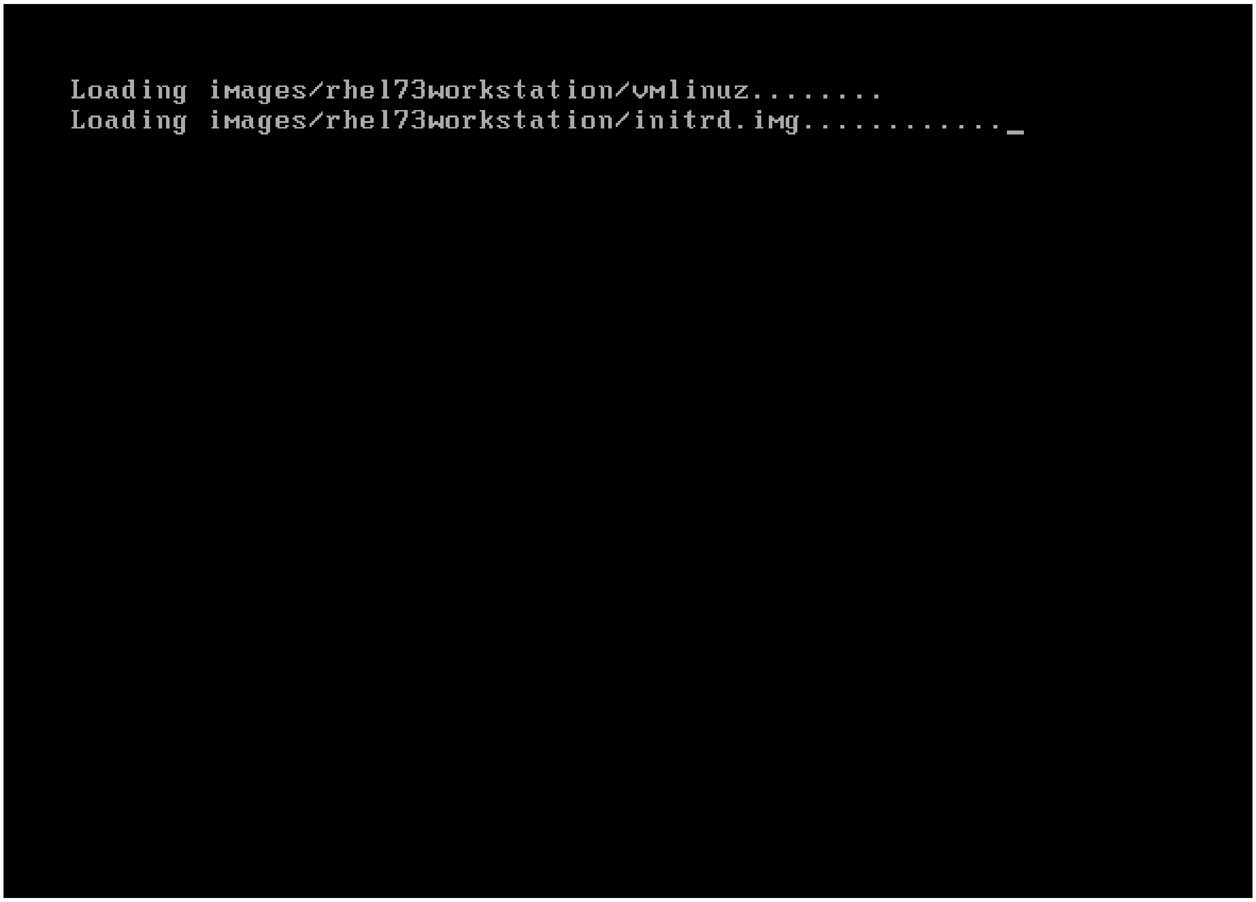


Linux Desktop Builds

Linux Desktop 6
Linux Desktop 7
Linux Desktop 6 - Interactive (ESD Only)
RHEL7 Workstation Blank - ESD ONLY
< Back to Main Menu

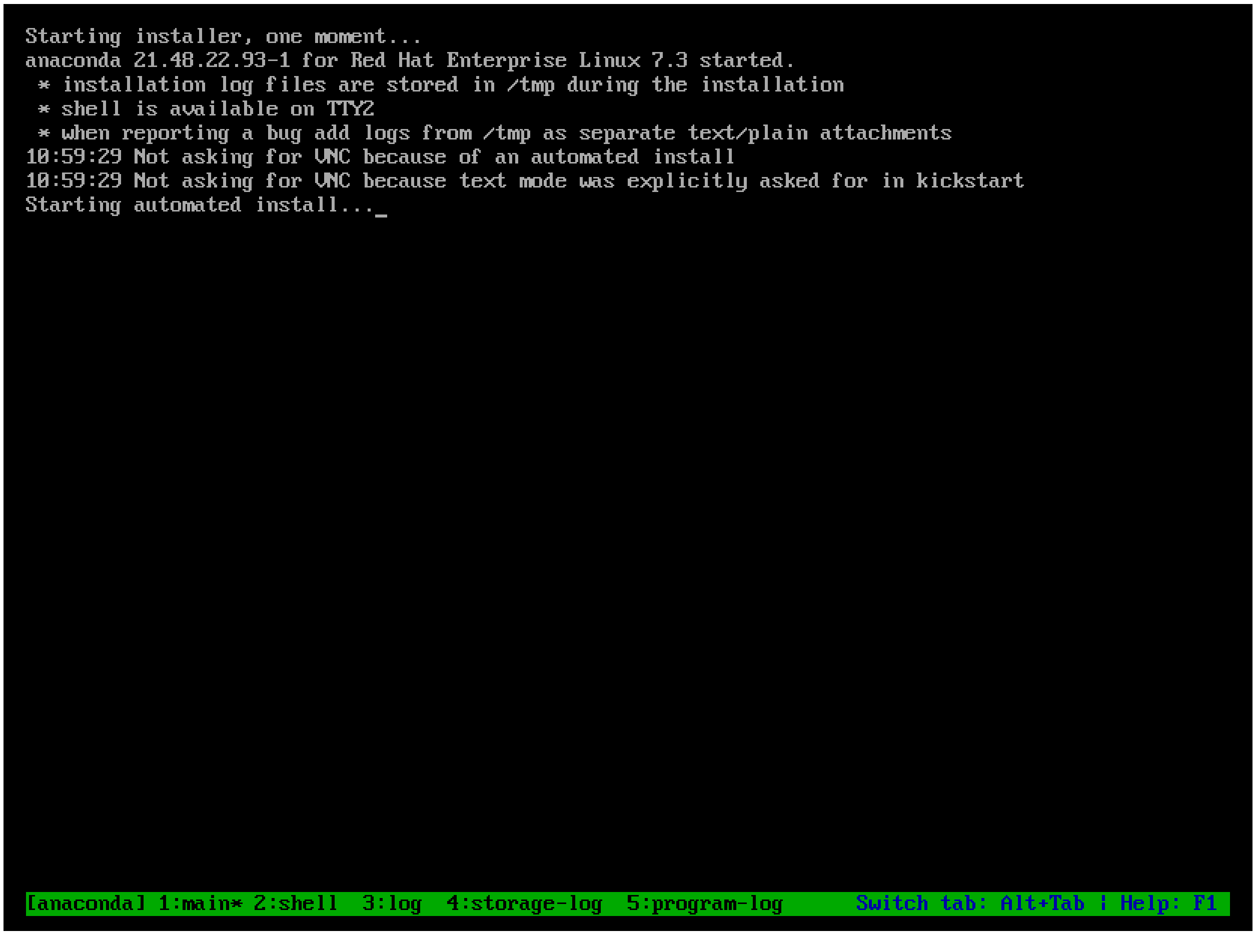
Password required
```
*****************************
```

If the build starts you'll see a loading screen like this one:



```
Loading images/rhel73workstation/vmlinuz........
Loading images/rhel73workstation/initrd.img............_
```

Followed by the Red Hat installer running automatically:



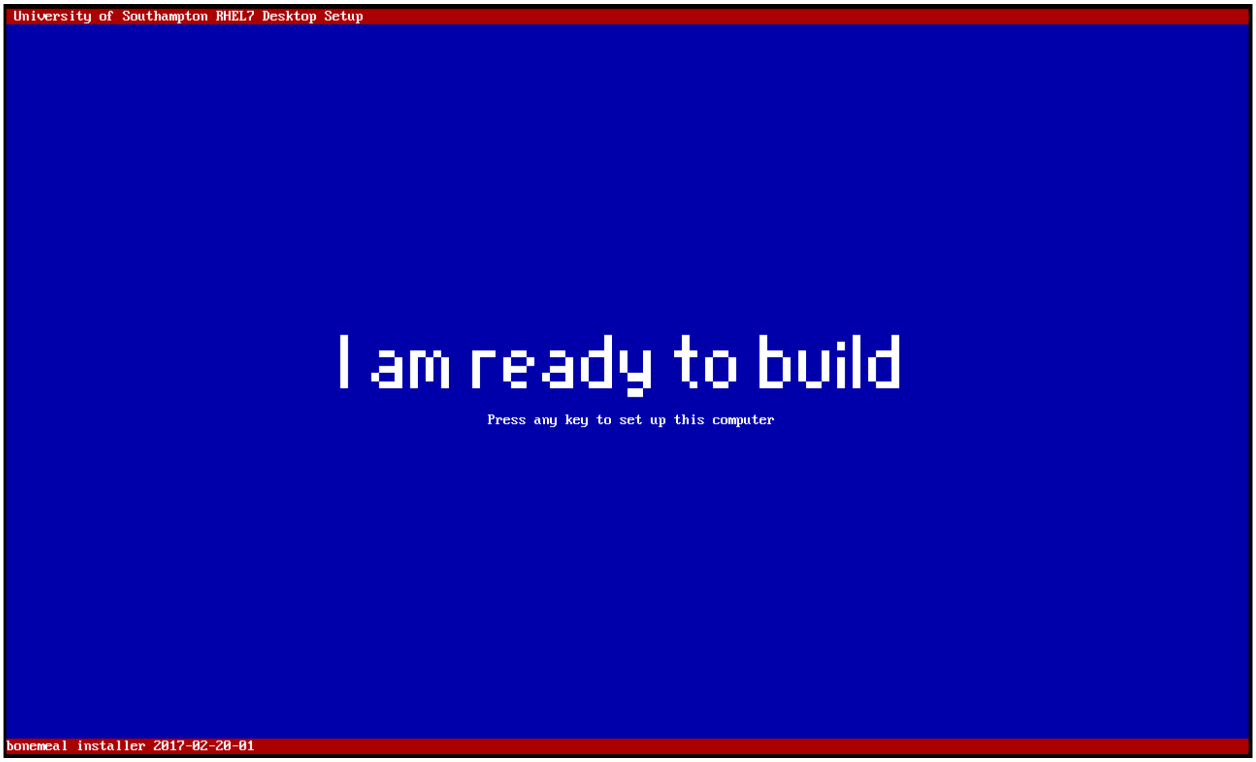
```
Starting installer, one moment...
anaconda 21.48.22.93-1 for Red Hat Enterprise Linux 7.3 started.
 * installation log files are stored in /tmp during the installation
 * shell is available on TTY2
 * when reporting a bug add logs from /tmp as separate text/plain attachments
10:59:29 Not asking for VNC because of an automated install
10:59:29 Not asking for VNC because text mode was explicitly asked for in kickstart
Starting automated install..._
```

```
[anaconda] 1:main* 2:shell  3:log  4:storage-log  5:program-log      Switch tab: Alt+Tab | Help: F1
```

The installation will take between 10 and 20 minutes. During this time you don't need to watch the computer, its fully automatic.

8.3 University installer

Once the Red Hat installer is finished the system will reboot and it will display a message telling you that the University installer has started and is ready to be used:



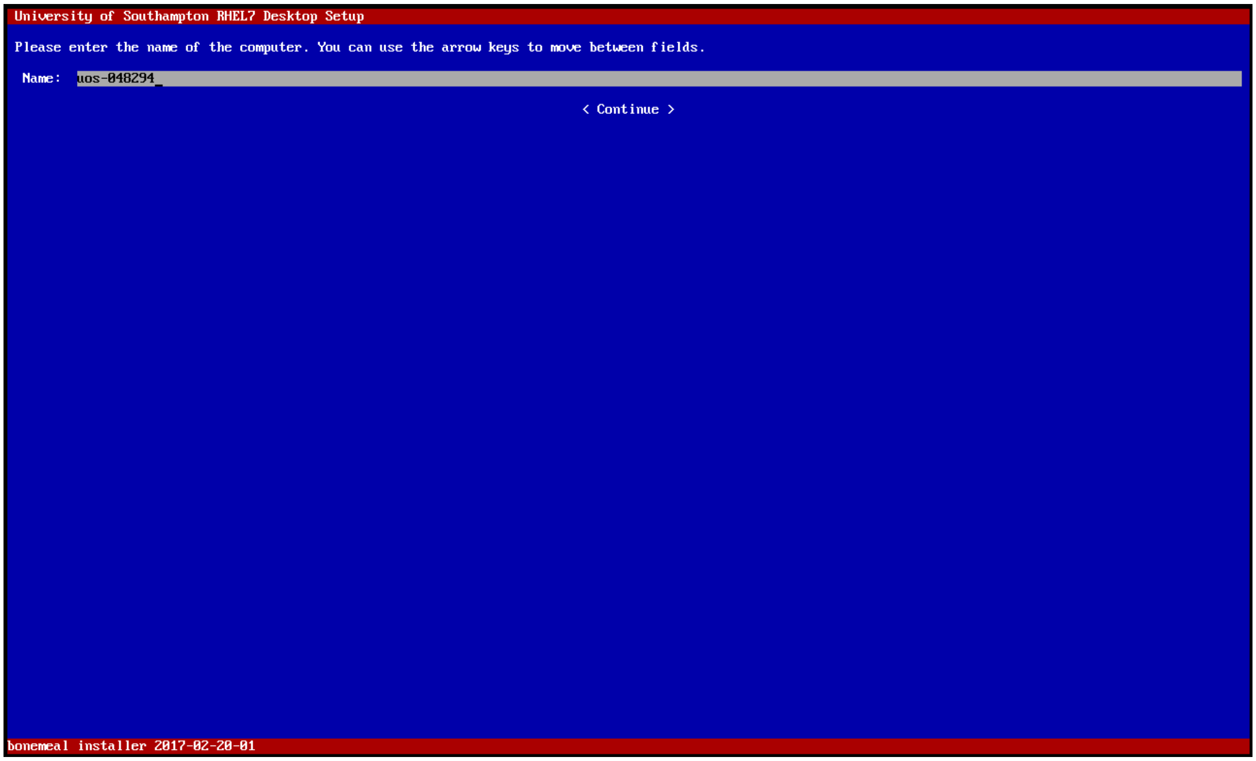
University of Southampton RHEL7 Desktop Setup

I am ready to build

Press any key to set up this computer

bonemeal installer 2017-02-20-01

Press any key to start the installer and then enter the computer name if it was not automatically detected:



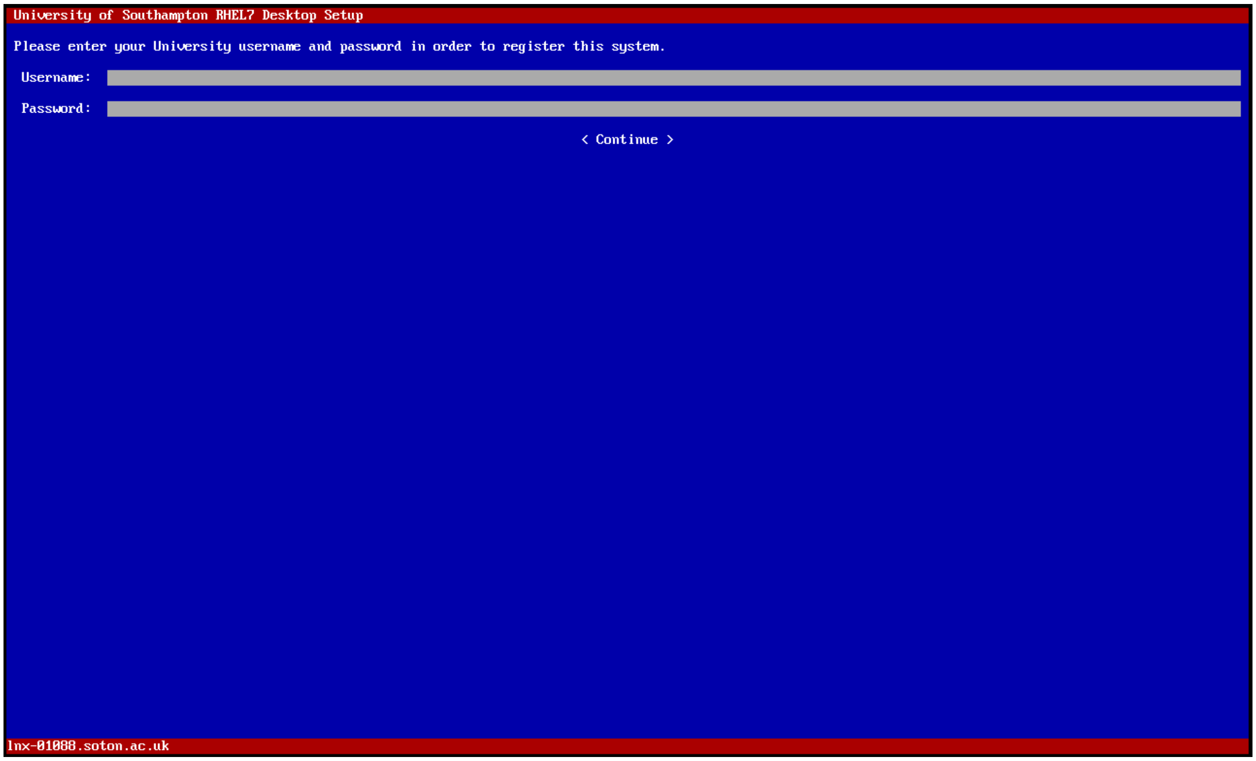
University of Southampton RHEL7 Desktop Setup

Please enter the name of the computer. You can use the arrow keys to move between fields.

Name: uos-048294

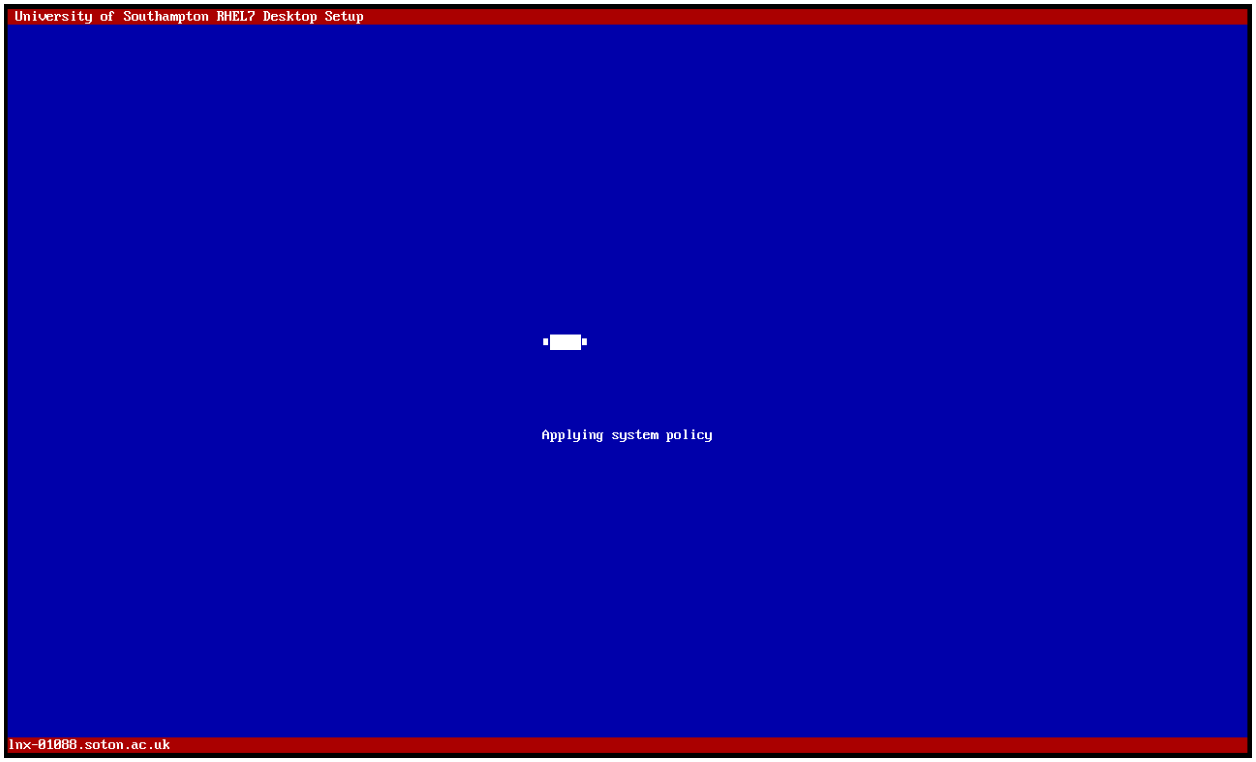
bonemeal installer 2017-02-20-01

You then need to enter your university username and password. The account must be within the `jfStaff` group - so don't use `adm` accounts, use your normal account.:



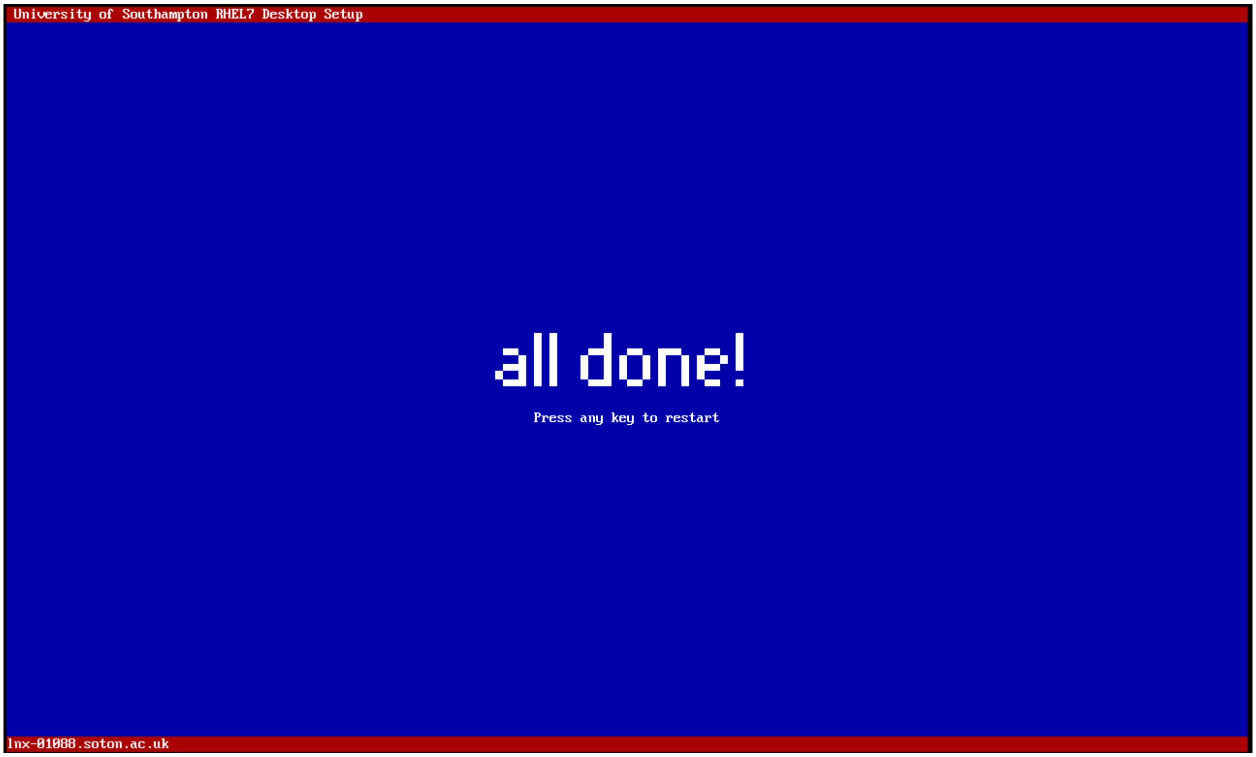
```
University of Southampton RHEL7 Desktop Setup

Please enter your University username and password in order to register this system.

 Username:

 Password:

                                   < Continue >

lnx-01088.soton.ac.uk
```

The University installer will then complete all its tasks automatically without requiring any further input. It can take between 5 and 15 minutes for this to finish, dependening on the speed of the hard drive:



```
University of Southampton RHEL7 Desktop Setup

                              Applying system policy

lnx-01088.soton.ac.uk
```

Once complete the installer will show "all done" and you can restart to use the new Linux desktop by pressing any key:



```
University of Southampton RHEL7 Desktop Setup

all done!

Press any key to restart

lnx-01088.soton.ac.uk
```

8.4 Post-installation tasks

Once the system has rebooted you might want to grant additional permissions to the user for whom you built the workstation for. To do so, logon to the system and use *Desktop Manager* to change *Permissions*. Your account must be within the `linuxadm` or `linuxsys` Linux groups to do this.

CHAPTER 9

Migration Guide

Note: This guide is intended for iSolutions staff only.

9.1 Introduction

This guide is intended to assist you migrating a customer's workstation from either RHEL5 or RHEL6 to our current RHEL7 platform. Before you start, you should make sure that you have a USB disk with no data on it that you can use to store data on the customer wishes to keep.

9.2 Migration outline

- Check for non-backed up data in /local/scratch/
- Copy data from /home/ to the USB drive
- Copy data from /local/scratch/ to the USB drive
- Check for secondary hard drives in the system
- Disconnect any secondary hard drives
- Install RHEL7
- Reconnect secondary hard drives
- Set up secondary hard drives to be automatically mounted
- Copy data back from the USB drive to /local/scratch/
- Copy data back from the USB drive to /home/
- Copy home directory data back

9.3 Check for non-backed up data in /local/scratch/

Users will probably want you to back up the data that is in `/local/scratch/` on the workstation. Although this data is not backed up normally, and is 'scratch' space we will still back it up to make things easier.

Ask the user if they have data they wish to keep in `/local/scratch`, and check if there is any other user data in `/local/scratch/` as well. If there is, it makes sense to back it up.

Do not check for data in `/data` - this is likely a second hard drive, which we will come onto later.

9.4 Attach the USB disk

Ask the user to log out of the system and ensure nobody else is logged in. Then login on the console and gain root. To switch to the console type `Ctrl+Alt+F3`.

Now plug in the USB disk you're going to use to store data on during the migration. You should then run the command `lsscsi` to list the attached storage devices. If lsscsi is not installed, installed it with:

```
yum install lsscsi
```

You can then run it like so:

```
lsscsi
```

And you should get an output somewhat similar to this:

```
[0:0:0:0]    disk    ATA      KINGSTON SA400S3 71E0  /dev/sda
[1:0:0:0]    cd/dvd  TSSTcorp CDDVDW SH-224BB  SB00  /dev/sr0
[2:0:0:0]    disk    Seagate  Expansion        9300  /dev/sdb
```

As you can see from the above, the USB drive (in this case a Seagate USB drive) is listed and it is available at the path `/dev/sdb`. If you've already set up the disk to be used by Linux systems then you can go ahead and mount the drive. We'll create a place to mount it:

```
mkdir /mnt/migrate
```

And then mount it:

```
mount /dev/sdb1 /mnt/migrate
```

9.5 Copy data

Now you'll want to use `rsync` to copy the data from the local system to the USB hard drive. We'll run it twice, once for `/home` and the second time for `/local/scratch/`. Here are the commands you'll want to run:

```
rsync -av --progress /home/ /mnt/migrate/home/
rsync -av --progress /local/scratch/ /mnt/migrate/scratch/
```

You can run these commands again to make sure all changes have been copied as they 'mirror' the data and only copy changes as needed. These commands will likely take a long time to run dependent on the speed of the hard drives and the amount of data.

9.6 Secondary hard drives

Sometimes a workstation will have a second or even a third physical disk installed. We don't have to back up this data as the installation for RHEL7 won't touch these disks - the data will be retained. However, it is best practice to disconnect these drives 'just in case'. If its easy to open the case and disconnect secondary hard drives, do so (when the power is off of course!) so as to prevent any chance of data on these disks from being lost.

Make a note as to how many of these drives there are, and where they are currently mounted. You can get a list of physical drives with `lsscsi`:

```
lsscsi
```

and you can get a list of mounted partitions with `df`:

```
df -h
```

This will let you figure out what drives are there, and what mount points to add once you've installed RHEL7. Make sure to write down the full path to the disk, e.g. it will probably be `/dev/sdb1` for the device path. You'll also want to make sure you write down the file system type, hopefully it will be `ext4`.

9.7 Install RHEL7

Once you've done the above steps, power the machine off, and unplug the USB hard disk. Then power it back on and follow the *Installation* guide.

9.8 Reconnect secondary hard drives

Once you've installed RHEL7 you should power the machine off again and reconnect any hard drives you previously disconnected. You can then power the machine back on and reconnect them. Log in and gain root, and then find a list of the new drives:

```
lsscsi
```

You should then re-create the directories where you want to mount the drives. In nearly all cases this will be `/data` so just run:

```
mkdir /data
```

Now you'll need to edit the file system tab (`fstab`) to add a record so the drive is mounted at startup. Edit `/etc/fstab` in the editor of your choice and add the following:

```
/dev/sdb1 /data ext4 defaults 0 0
```

Change this line to match what you need it to - .e.g change `/dev/sdb` to be the device path you wrote down in the earlier steps. Change `/data` to be wherever the disk should be mounted. And change `ext4` to whatever file system is in use (and you wrote down earlier). In nearly all cases though you probably won't need to change anything.

Once that is done, save and exit the file, and run:

```
mount -a
```

Now check the disk is mounted:

```
df -h
```

9.9 Copy data back

The last step is to copy data back onto the workstation. You'll have to plug in the USB drive in again, and then work out what it got attached as:

```
lsscsi
```

And you should get an output somewhat similar to this:

```
[0:0:0:0]    disk    ATA      KINGSTON SA400S3 71E0  /dev/sda
[1:0:0:0]    cd/dvd  TSSTcorp CDDVDW SH-224BB  SB00  /dev/sr0
[2:0:0:0]    disk    Seagate  Expansion        9300  /dev/sdb
```

As you can see from the above, the USB drive (in this case a Seagate USB drive) is listed and it is available at the path `/dev/sdb`. Create the place we'll mount it:

```
mkdir /mnt/migrate
```

And then mount it:

```
mount /dev/sdb1 /mnt/migrate
```

Now we can copy data back. Start with the `/local/scratch/` directory and use `rsync` again to copy back:

> rsync -av –progress /mnt/migrate/scratch/ /local/scratch/

You can then recover the `/home` directory data. You probably should not recover the data directly though. In most cases, users will be moving from GNOME 2 to GNOME 3, and starting with a fresh home directory makes more sense. If a user insists they want their original home directory, feel free to restore it, but it can lead to problems, and so you should recommend that they do not.

Either restore the data into /local/scratch/home/ like so:

```
rsync -av --progress /mnt/migrate/home/ /local/scratch/home/
```

Or restore individual directories for users (not recommended):

> rsync -av –progress /mnt/migrate/home/<username>/ /home/<username>/

CHAPTER 10

Permissions

10.1 Standard permissions

All members of the University of Southampton can log on to any Linux Desktop. Once logged in you are granted all normal Linux account rights, and in addition you may perform the following actions:

- Can install software packages via *Desktop Manager*
- Can install software packages via GNOME Software
- Can mount and umount file systems via `sudo mount` (See *Network storage*)
- Mount a file systems via GNOME disk management
- Can manage NVIDIA graphics settings via `sudo nvidia-settings`
- Can reboot/poweroff/hibernate/suspend the computer
- Can run the following commands: `reboot`, `poweroff`, `halt`
- Can start a backup with `sudo drone backup now`
- Can check the backup status with `sudo drone backup status`

10.2 Additional permissions

There are four user groups on each workstation which grant additional privileges:

10.2.1 SSH Access

Users in the group `users` are granted the privilege of being able to logon to the system via SSH from anywhere within the university network.

10.2.2 Administrator

Users in the group sys are considered administrators. Although they lack full root access they are granted several privileges. They can use sudo to run the following commands as root:

- yum - for installing software packages
- rpm - for installing local RPM packages
- pip - for installing Python packages
- cpan - for installing Perl modules
- gem - for installing Ruby gems (packages)

They are also granted permissions via PolicyKit to do the following:

- Manage local storage via GNOME disks (or any udisks2 application)
- Full control over power management
- Change locale settings
- Remove software packages
- Update the system software
- Trigger an offline system update
- Manage the date and/or time
- Manage printers (including adding printers)
- Manage the network settings
- Manage tuned
- Reinstall the VirtualBox kernel module (See *Virtualisation*)
- Set the default version of java/javac (See *Java*)

iSolutions are more than happy to grant additional privileges to these users upon request.

10.2.3 Virtual Box

Users in the vboxusers group can utilise USB devices in Virtual Box and can reinstall the VirtualBox kernel module.

10.2.4 Root access

Users in the wheel group are granted full root access via sudo and are granted all privileges via policykit. Only members of iSolutions can grant access to this group and is done so rarely.

10.3 Granting permissions

You can use *Desktop Manager* to add and remove users from groups. Local administrators (users in the group sys) can add and remove users from the following groups:

- SSH access (users)
- Administrators (sys)

- VirtualBox users (`vboxusers`)

Only iSolutions staff in the `linuxadm` or `linuxsys` groups can add or remove users from the `wheel` group.

CHAPTER 11

Remote access

11.1 SSH

You can connect to your Linux desktop via the SSH protocol. To do so your user account needs to be in the `users` group. Read the *Permissions* page for more details about permissions, or use *Desktop Manager* to add yourself to the SSH group.

The address to connect to will be of the form:

```
uos-NNNNN.clients.soton.ac.uk
```

If you don't know what your computer's "UOS" number is, you can find out by either opening *Desktop Manager* or by opening a terminal and typing:

```
hostname
```

For example if your computers UOS name were `uos-57292` you would connect to the address `uos-57292.clients.soton.ac.uk`. You can then login with your normal university username and password.

CHAPTER 12

Desktop environments

12.1 GNOME 3

GNOME 3 is the default desktop environment on university Linux desktops. It is the most feature complete and useful desktop and as such as we highly recommend using it.

GNOME 3, like many recent desktop environments, does not use the classic Windows style task bar model, or the Mac OS X style dock model. It can however be heavily customised by the *GNOME Tweak Tool* and *GNOME Extensions*.

12.2 Xfce 4

XFCE is a lightweight alternative to GNOME, whilst still utilising a lot of the core components of GNOME. It can be heavily customised and is considered a more traditional desktop environment. If you do not like GNOME 3 then we recommend using XFCE instead.

You can use *Desktop Manager* to install XFCE, or use the following command in a terminal:

```
sudo yum groupinstall xfce-desktop
```

12.3 KDE Plasma

KDE Plasma is the latest version of the K Desktop Environment, an alternative desktop platform based on the Qt framework. Unlike KDE 3, the KDE Plasma environment is not well regarded, and it lacks a lot of features and maturity of both GNOME and XFCE. Although available to install we do not recommend using KDE Plasma.

You can use *Desktop Manager* to install KDE, or use the following command in a terminal:

```
sudo yum groupinstall kde-desktop-environment
```

12.4 MATE

MATE is a fork of the GNOME 2 project, and as such it is essentially an updated GNOME 2 desktop environment. If you liked GNOME 2, and wish to continue using it, then MATE may suit you. The latest version of MATE - 1.16 - is available and despite being based on GNOME 2 has been largely rewritten in GTK3.

You can use *Desktop Manager* to install MATE, or use the following command in a terminal:

```
sudo yum groupinstall kde-desktop-environment
```

12.5 i3

i3 is a tiling window manager similar to wmii. It is not a full desktop environment and it is intended for advanced users. Unless you have experience with ultra lightweight tiling window managers we do not recommend using i3.

You can use *Desktop Manager* to install i3, or use the following command in a terminal:

```
sudo yum install i3
```

12.6 Others

Several other desktops are available:

- Cinnamon: `sudo yum install cinnamon-desktop`
- LXDE / LXQt: `sudo yum install lxqt-session lxqt-panel lxqt-config lxqt-powermanagement lxqt-wallet lxqt-policykit`

Several other window managers are available:

- xmonad: `sudo yum install xmonad`
- fluxbox: `sudo yum install fluxbox`
- openbox: `sudo yum install openbox`
- IceWM: `sudo yum install icewm`
- Matchbox: `sudo yum install matchbox-window-manager`
- WindowMaker: `sudo yum install WindowMaker`
- spectrwm: `sudo yum install spectrwm`
- fvwm: `sudo yum install fvwm`
- pekwm: `sudo yum install pekwm`
- vtwm: `sudo yum install vtwm`

CHAPTER 13

Virtualisation

13.1 VirtualBox

iSolutions recommends the use of VirtualBox for creating and running virtual machines on the linux desktop platform. VirtualBox is designed for a multi user environment, unlike KVM/libvirt which runs everything as root.

You can install the latest VirtualBox with the following command:

```
sudo yum install VirtualBox-5.1
```

Older versions are available but we recommend you install the latest.

Once installed you can start VirtualBox and start creating virtual machines straight away! We recommend you store your virtual machine disks in the `/local/scratch/<username/` directory - see *Local storage* for more info.

13.2 Rebuilding the kernel module

After a `kernel` update is installed you might find that VirtualBox no longer works and generates an error similar to `Kernel driver not installed`. To fix this you must run the following command in a terminal:

```
sudo /usr/lib/virtualbox/vboxdrv.sh setup
```

To run the above command you must be in the `sys` or `vboxusers` group. See *Permissions* for more information.

13.3 VirtualBox user group

In previous versions of VirtualBox anybody who wanted to use the software had to be in the `vboxusers` group. This is no longer the case and membership of this group is only required if:

- You want to be able to rebuild the kernel module without being in `sys`

- You want to be able to use USB passthrough devices

See *Permissions* for more information.

CHAPTER 14

Firewall

From RHEL7 (Red Hat Enterprise Linux Version 7) onwards you can now manage the firewall of your workstation provided you are a member of the `sys` users group. See *Permissions* for further information on groups.

The firewall is managed by the `firewalld` utility. To manage the firewall you need to start the graphical tool "Firewall Config". You can then use this GUI tool to make changes.

Please only make changes to the firewall if absolutley necessary. The defaults are probably all you need.

CHAPTER 15

GNOME Extensions

GNOME 3 features a unique extension system which allows you to install various add on packages within GNOME. These extensions can be used to fix a lot of the behaviour of GNOME 3 that many people do not like.

When you first login to a RHEL7 (Red Hat Enterprise Linux version 7) desktop you will be logged into 'GNOME Classic' which is GNOME 3 with a lot of extra GNOME extensions.

15.1 Finding and installing extensions

Open the Firefox web browser and navigate to extensions.gnome.org

The website itself is used to find and install extensions.

Once installed you can open the `GNOME Tweak Tool` to configure extensions.

15.2 Recommended extensions

iSolutions recommend the following extensions which will enhance GNOME 3:

- Dash to Dock
- TopIcons
- Sound input & output device chooser
- Places status indicator
- Log out button
- Trash button

For laptops:

- Battery Percentage
- Refresh Wifi Connections

CHAPTER 16

Environment modules system

Most of the scientific and research software provided by iSolutions uses the environment modules system. Most if not all of the software on the IRIDIS super computer also uses the environment module system.

The modules system is a way to dynamically alter your environment (e.g. variables in your terminal session) in a ‘modular’ way. An application specifies a ‘module file’ which contains code to modify the shell so that the application works. You can then ‘load’ the module which uses the module file.

16.1 How to load a module

First you have to install some software which makes use of the modules system, for example you could install PyPy 5.6:

```
sudo yum install pypy256
```

Once the package is installed you can switch into the module like so:

```
module load pypy/5.6
```

Once loaded you can use the `pypy` binary directly.

16.2 How to unload a module

Just replace `module load` with `module unload`:

```
module unload pypy/5.6
```

16.3 List available modules

You can list all the modules installed with:

```
module avail
```

16.4 Show the help for the module

Each module should have some help text, use this command to show it:

```
module help pypy/5.6
```

16.5 List loaded modules

You can list the modules in use right now type:

```
module list
```

CHAPTER 17

Software collections (SCL)

Sofware collections - or SCL - is a collection of 'add-on' software packages created and maintained by Red Hat. They were created in order to deliver more up to date versions of software to customers on Red Hat Enterprise Linux which typically does not update software "mid-life" of a product. Via SCL Red Hat is able to provide more recent stable versions of software for customers to use without affecting the stability and security of the base product.

Due to our education licence all SCL software is available to users of our linux desktops. More information about all the available packages can be found on the dedicated software collections website.

17.1 How to install SCL packages

SCL packages are normal rpm software packages and thus can be installed via the usual tools, see *Installing software* for more information. Typically the SCL packages will contain 'rh' in the name, but not all do.

17.2 How to use SCL packages

Once you have installed an SCL package you must first 'enable' its use and run a program with the package enabled. For example:

```
scl enable rh-python35 bash
```

This 'enables' the rh-python35 package (Python 3.5) and then runs the command `bash`. The `bash` command is started with some environment variables changed so that the SCL software is then available, in a similar way to how *Environment modules system* work.

You can also enable two or more environments at the same time like so:

```
scl enable sclone scltwo bash
```

In the above example both `sclone` and `scltwo` are enabled.

17.3 Using SCL without the `scl` command

Unlike the environment modules system the binaries of the programs do not have a `PREFIX` set so they can locate shared libraries (shared/dynamic objects) without setting the `LD_LIBRARY_PATH` variable. This is set automatically by the `scl enable` command.

You can however source a script instead of having to use the `scl` command. Each SCL package is installed into `opt`:

```
/opt/rh/<package-name>/
```

Within that directory there is a script named `enable` which you can `source`:

```
source /opt/rh/<package-name>/enable
```

For example this is how to source Python 3.5:

```
source /opt/rh/rh-python35/enable
```

CHAPTER 18

Python

Python is a popular and versatile programming language used in many scientific disciplines across the university. It is by far the most popular language in use by staff at Southampton and is the most used tool on Windows desktops too!

The university Linux desktop platform has a large number of Python implementations for you to choose from. We've worked hard to try to provide the options you might need and granted you the privileges needed to install packages as required.

Note: To install python modules via `sudo pip` you need to be in the Administrators group. See *Permissions* for more information. You don't need to be in this group to use the `conda` command. You can also use `pip` directly, without `sudo`, and install packages in your home directory.

18.1 List of available implementations

- CPython
  - RHEL system python - 2.7.5
  - Miniconda (Anaconda) - 2.7, 3.6
  - *IUS* packages - 3.4.6, 3.5.3, 3.6.0
  - *SCL* packages - 2.7.8, 3.3.2, 3.4.2, 3.5.1
  - *EPEL* package - 3.4.5
- PyPy
  - PyPy 5.6 - 2.7.12
  - PyPy3 5.5-alpha - 3.3
- Jython
  - *SCL* Jython 2.7

You can use *Desktop Manager* to install the various options, or read below for the `yum` commands to use instead.

18.2 Which implementation should I use?

- If you want to use Python 2, and you don't need `conda` packages, then use the RHEL system Python, and use `pip` to install packages.
- If you want to use Python 3, and you don't need `conda` pacakges, then use the IUS Python 3.6 package and use `pip3.6m` to install pacakges
- If you need `conda` packages (Anaconda Python packages) then use miniconda

18.3 RHEL system Python

Unless you need Python 3 or `conda` packages then we recommend you use the system python in `/usr/bin/python`. This is supported by Red Hat and kept up to date with security and bug fixes.

You can install packages by running `sudo pip` eg:

```
sudo pip install numpy
```

18.4 IUS Python

The *IUS* repository provides Python 3 packages for Red Hat Enterprise Linux. If you need to use Python 3 then we recommend you use the *IUS* Python packages. Several versions are available for install:

- Python 3.4 - `sudo yum install python34u python34u-pip`
- Python 3.5 - `sudo yum install python35u python35u-pip`
- Python 3.6 - `sudo yum install python36u python36u-pip`

You can then use Python via the following paths to the binary:

- Python 3.4 - `/usr/bin/python3.4`
- Python 3.5 - `/usr/bin/python3.5`
- Python 3.6 - `/usr/bin/python3.6`

The version of Python in `/usr/bin/python3` depends on the order the *IUS* packages are installed, so we don't recommend you use that path.

You can install packages via `sudo pip`:

- Python 3.4 - `sudo pip3.4`
- Python 3.5 - `sudo pip3.5`
- Python 3.6 - `sudo pip3.6`

For example, to install `numpy` on *IUS* Python 3.6:

```
sudo pip3.6 install numpy
```

18.5 PyPy

PyPy is a just-in-time (JIT) compiler for Python which aims to be compatible with the standard CPython implementation. Using PyPy often yields significant performance benefits.

To install PyPy run the following command:

```
sudo yum install pypy256
```

This installs PyPy 5.6 which is compatible with CPython 2.7.12.

To install PyPy3 run the following command:

```
sudo yum install pypy3355
```

This installs PyPy3 5.5-alpha which is compatible with CPython 3.3.5.

To run PyPy you can either use the following paths:

- `/usr/bin/pypy56` - PyPy 5.6 (Python 2.7.12)
- `/usr/bin/pypy3355` - PyPy 5.5-alpha (Python 3.3.5)

Or you can use the `module` system:

- `module load pypy/5.6` - PyPy 5.6 (Python 2.7.12)
- `module load pypy/3.3-5.5` - PyPy 5.5-alpha (Python 3.3.5)

Once you've loaded the module you can use the `pypy` command directly and it will correspond to the version of pypy you chose to load.

You can install packages with `pip`:

- `sudo /local/software/pypy/5.6/bin/pip` - PyPy 5.6 (Python 2.7.12)
- `sudo /local/software/pypy/3.3-5.5/bin/pip3` - PyPy 5.5-alpha (Python 3.3.5)

For example, to install `numpy` on PyPy 5.6:

```
sudo /local/software/pypy/5.6/bin/pip install numpy
```

18.6 Miniconda (Anaconda)

Anaconda, and its `conda` package manager, is an alternative to the `pip` package manager (although the developers insist it complements pip and solves different problems).

Anaconda, conda and miniconda are not designed for "system-wide" use, they are intended for individual users to download and install for just that one user. Better multi user support is planned, but as of March 2017, is not yet available.

To use `conda` you don't need to download and install Anaconda or miniconda yourself, instead you can get started by installing `miniconda` which just contains `conda` and `python`:

```
sudo yum install miniconda
```

Once installed you can use `conda` to create a new environment within your home directory with whatever version of Python and whichever Python packages you need.

You should start by creating an environment, e.g:

```
conda create -n yourenvname python=x.x
```

You specify the version of python you want with the `python=x.x` flag, but this is optional and if omitted conda will use the version of Python shipped with `miniconda` which at the time of writing is Python 3.6.0.

You can specify at creation time the packages you want installed. For example, to install the entire anaconda set of packages you can do the following:

```
conda create -n yourenvname python=3.6 anaconda
```

You can then use your new environment like so:

```
source activate yourenvname
```

And you can then stop using it like so:

```
source deactivate
```

You can install additional packages with `conda`:

```
conda install -n yourenvname [package]
```

And if you want to delete an environment do the following:

```
conda remove -n yourenvname -all
```

18.7 SCL Python

Note: The *SCL* python33 package conflicts with the *IUS* Python packages. You cannot have both versions installed at the same time. To install the *SCL* python33 package you must first remove the *IUS* Python packages. In any case we strongly recommend you use the *IUS* packages rather than *SCL*.

Red Hat provides several CPython packages as part of its "Software Collections" system. These packages are generally older than the *IUS* packages and are more difficult to use - they require the use of the `scl` command. At the time of writing the following versions are available:

- Python 2.7.8 - `sudo yum install python27 python27-python-pip`
- Python 3.3.2 - `sudo yum install python33`
- Python 3.4.2 - `sudo yum install rh-python34 rh-python34-python-pip`
- Python 3.5.1 - `sudo yum install rh-python35 rh-python35-python-pip`

Once installed you can't use python until you use the `scl` command which is somewhat like the environment module system:

- Python 2.7.8 - `scl enable python27 bash`
- Python 3.3.2 - `scl enable python33 bash`
- Python 3.4.2 - `scl enable rh-python34 bash`
- Python 3.5.1 - `scl enable rh-python34 bash`

Once you've run the scl command then the python command will now be the version of Python you requested. The pip command will also be updated for the *SCL* python, but it won't work unless you use a special sclsudo command we've created. So to install packages you should run:

```
sclsudo pip install numpy
```

18.8 EPEL Python

Note: The EPEL python 3.4 package conflicts with the *IUS* Python 3.4 package. You cannot have both versions installed at the same time. To install the EPEL python you must first remove the *IUS* Python 3.4 packages. In any case we strongly recommend you use the *IUS* packages rather than EPEL.

Another alternative Python 3 package is provided by :doc'epel'. We recommend that you use the *IUS* packages instead since the EPEL Python package is now quite out of date. If you do want to use it, install it like so:

```
sudo yum install python34 python34-pip
```

You can then use the package with the binary path:

```
/usr/bin/python3.4
```

and you can install packages with pip:

```
sudo /usr/bin/pip3.4 install numpy
```

18.9 Jython

Jython is an implementation of Python running on the Java virtual machine (JVM). Red Hat have provided a packaged version of Jython as part of their Developer Toolset 4 product. To install it run this command:

```
sudo yum install devtoolset-4 devtoolset-4-jython
```

Then run the scl command to enable it:

```
scl enable devtoolset-4 bash
```

You can then run jython directly:

```
jython
```

CHAPTER 19

C and C++

C is a general-purpose, low level, imperative computer programming language, supporting structured programming, lexical variable scope and recursion, while a static type system prevents many unintended operations. C++ is an extension of C with object-oriented features and a much larger standard library.

19.1 List of compilers

Several C and C++ compilers are available on the Linux desktop platform:

- GCC (GNU compiler collection)
  - v4.8 - Red Hat's built in GCC
  - v4.9 - part of *RHDT* 3
  - v5.3 - part of *RHDT* 4
  - v6.2 - part of *RHDT* 6
- ICC/ICPC (Intel compiler suite)
  - 2017 Update 2
- Clang (LLVM C/C++ compiler)
  - v4.0.0
  - v3.9.1
  - v3.4.2 from the *EPEL* project
- PGI (NVIDIA Portland Group Compiler Suite)
  - 17.1

19.2 GCC

Several versions of GCC are available. The system gcc - the one used to build Red Hat Enterprise Linux 7 - is version 4.8. You can install it like so:

```
sudo yum install gcc gcc-c++
```

Later versions are available as part of the *RHDT* bundles:

- v4.9: `sudo yum install devtoolset-3-gcc devtoolset-3-gcc-c++`
- v5.3: `sudo yum install devtoolset-4-gcc devtoolset-4-gcc-c++`
- v6.2: `sudo yum install devtoolset-6-gcc devtoolset-6-gcc-c++`

Once you have installed the packages you need to use *SCL* to use the updated version of gcc like so:

```
* v4.9: ``scl enable devtoolset-3 bash``
* v5.3: ``scl enable devtoolset-4 bash``
* v6.2: ``scl enable devtoolset-6 bash``
```

Once those commands are run then running 'gcc' will run the version you requested.

See the *Software collections (SCL)* document for more information on using *SCL*.

19.3 Intel

Intel's C and C++ compiler is part of the Intel Parallel Studio XE product. This is available to you as a member of the University. At the time of writing the latest version - 2017 Update 2 - is available. To install it you can use the following command:

```
sudo yum install intel-parallel-studio-2017u2
```

This installs all of the components of the Cluster Edition of the Intel Parallel Studio. To use the Parallel Suite you must first load the environment module:

```
module load intel/2017u2
```

Once loaded all of the environment modules are set such that you should be able to run the `configure` script (or similar mechanism) and it should use the Intel compilers. You can also use `icc`, `icpc` and `ifort` directly.

See *Environment modules system* for more information on using the module system.

19.4 LLVM Clang

Clang is the compiler from the LLVM project. To use it first install the latest version:

```
sudo yum install llvm400
```

The LLVM package includes:

- LLVM core libraries
- Clang
- compiler-rt

- LLDB (LLVM debugger)
- LLD (LLVM linker)

Once installed you should use the *Environment modules system* to use clang itself:

```
module load llvm/4.0.0
```

See *Environment modules system* for more information on using the module system.

19.5 NVIDIA PGI Compilers

The portland group (PGI) compilers, now owned by NVIDIA, are a series of high performance C, C++ and Fortran compilers which are heavily used within high performance computiing. To use the PGI compilers first install the latest version:

```
sudo yum install pgi171
```

Once installed you should use the *Environment modules system* to use the compilers:

```
module load pgi/17.1
```

You can then use `pgcc` (the C compiler), `pgc++` (the C++ compiler) or `pgfortran` (the Fortran compiler) directly.

See *Environment modules system* for more information on using the module system.

CHAPTER 20

Fortran

Fortran is a general-purpose, imperative programming language that is especially suited to numeric computation and scientific computing. FORTRAN was developed in the 1950s making it one of the oldest languages still in use. It is often use for computational chemistry and fluid dynamics.

20.1 List of compilers

Several different compilers are available:

- gFortran (Part of the GNU compiler collection)
  - v4.8 - Red Hat's built in gFortran
  - v4.9 - part of *RHDT* 3
  - v5.3 - part of *RHDT* 4
  - v6.2 - part of *RHDT* 6
- NVIDIA Portland Group (PGI) Fortran
  - 17.1
- Intel Parallel Studio XE:
  - 2017 Update 2

20.2 GCC

Several versions of gFortran are available. The standard version, tied to the system GCC version, is v4.8 You can install it like so:

```
sudo yum install gcc-gfortran
```

Later versions are available as part of the *RHDT* bundles:

- v4.9: `sudo yum install devtoolset-3-gcc-gfortran`
- v5.3: `sudo yum install devtoolset-4-gcc-gfortran`
- v6.2: `sudo yum install devtoolset-6-gcc-gfortran`

Once you have installed the packages you need to use *SCL* to use the updated version of gfortran like so:

- v4.9: `scl enable devtoolset-3 bash`
- v5.3: `scl enable devtoolset-4 bash`
- v6.2: `scl enable devtoolset-6 bash`

Once those commands are run then running 'gfortran' will run the version you requested.

See the *Software collections (SCL)* document for more information on using *SCL*.

20.3 PGI Fortran

The portland group (PGI) compilers, now owned by NVIDIA, are a series of high performance C, C++ and Fortran compilers which are heavily used within high performance computiing. To use the PGI compilers first install the latest version:

```
sudo yum install pgi171
```

Once installed you should use the *Environment modules system* to use the compilers:

```
module load pgi/17.1
```

You can then use `pgfortran` (the Fortran compiler) directly, or one of the several version specific binaries:

- `pgf77`
- `pgf90`
- `pgf95`

See *Environment modules system* for more information on using the module system.

20.4 Intel

Intel's Fortran compiler - `ifort` - is part of the Intel Parallel Studio XE product. This is available to you as a member of the University. At the time of writing the latest version - 2017 Update 2 - is available. To install it you can use the following command:

```
sudo yum install intel-parallel-studio-2017u2
```

This installs all of the components of the Cluster Edition of the Intel Parallel Studio. To use the Parallel Suite you must first load the environment module:

```
module load intel/2017u2
```

Once loaded all of the environment modules are set such that you should be able to run the `configure` script (or similar mechanism) and it should use the Intel compiler. You can also use `ifort` directly.

See *Environment modules system* for more information on using the module system.

CHAPTER 21

Java

Java is a general purpose object oriented programming language and runtime. It is intended to let application developers “write once, run anywhere” through compiling Java code to ‘byte code’ which is then run on the Java virtual machine.

21.1 Java implementations

There are several implementations of Java available on the Linux desktop platform:

- Oracle - v1.6, v1.7, v1.8
- OpenJDK - v1.6, v1.7, v1.8
- IBM - v1.7, v1.8

We strongly recommend the use of either Oracle Java 1.8 or OpenJDK Java 1.8.

You can install the different versions via *Desktop Manager* or if you prefer here are the commands to run in a terminal to install them instead:

Oracle Java 1.6	`sudo yum install java-1.6.0-sun-devel`
Oracle Java 1.7	`sudo yum install java-1.7.0-oracle-devel`
Oracle Java 1.8	`sudo yum install java-1.8.0-oracle-devel`
OpenJDK Java 1.6	`sudo yum install java-1.6.0-openjdk-devel`
OpenJDK Java 1.7	`sudo yum install java-1.7.0-openjdk-devel`
OpenJDK Java 1.8	`sudo yum install java-1.8.0-openjdk-devel`
IBM Java 1.7	`sudo yum install java-1.7.1-ibm-devel`
IBM Java 1.8	`sudo yum install java-1.8.0-ibm-devel`

Sadly the Java packages do not use the *Environment modules system* or the *SCL* system, so you will have to use the full path to the `java` or `javac` binaries:

Oracle Java 1.6	`/usr/lib/jvm/java-1.6.0-sun.x86_64/bin/java`
Oracle Java 1.7	`/usr/lib/jvm/java-1.7.0-oracle/bin/java`
Oracle Java 1.8	`/usr/lib/jvm/java-1.8.0-oracle/bin/java`
OpenJDK Java 1.6	`/usr/lib/jvm/java-1.6.0-openjdk.x86_64/bin/java`
OpenJDK Java 1.7	`/usr/lib/jvm/java-1.7.0-openjdk/bin/java`
OpenJDK Java 1.8	`/usr/lib/jvm/java-1.8.0-openjdk/bin/java`
IBM Java 1.7	`/usr/lib/jvm/java-1.7.0-ibm/bin/java`
IBM Java 1.8	`/usr/lib/jvm/java-1.8.0-ibm/bin/java`

21.2 Setting the default system Java

Instead of having to use the above method to use a particular version of Java you may use the `alternatives` command to change the default version of Java in use. This will affect every user on the system so please only do this if you are sure you will not impact other users.

Note: To set the system wide default Java you need to be in the Administrators group. See *Permissions* for more information.

Run the following commands and follow the instructions to change the default:

```
sudo alternatives --config java
sudo alternatives --config javac
```

CHAPTER 22

TeX Live (LaTeX)

TeX and LaTeX are document production tools otherwise known as typesetting systems. TeX and LaTeX are used to produce high quality documents and books, especially within academia. LaTeX is used for producing scientific documents throughout the University.

TeX Live is a distribution which contains both TeX and LaTeX, among many other tools and programs.

22.1 Versions of TeX Live

There are two versions of TeX Live available:

- Tex Live 2013: `sudo yum install texlive`
- Tex Live 2016: `sudo yum install texlive2016`

The former version is packaged by Red Hat and does not include the `tlmgr` TeX package manager. As such we recommend you install TeX Live 2016 which is the latest version and it includes the package manager.

22.2 Using Tex Live 2016

TeX Live 2016 uses the *Environment modules system*. To use it open a terminal and run the following:

```
module load texlive/2016
```

Once loaded you can use all the normal TeX/LaTeX commands (and man pages).

22.3 Installing TeX modules

Note: To install TeX modules via `sudo tlmgr` you need to be in the Administrators group. See *Permissions* for more information. You can also install modules in your home directory if you prefer.

TeX Live 2016 comes with a package manager called `tlmgr`. You can install modules like so:

```
sudo tlmgr install <modulename>
```

If you prefer to install a module just for yourself, or if you don't have permission to use `sudo tlmgr`, run:

```
tlmgr --usermode install <modulename>
```

CHAPTER 23

R

R is an open source programming language intended for use within statistical computing and data analysis. It is not installed by default on the Linux desktop platform but it can be installed easily via the following command in a terminal:

```
sudo yum install R
```

23.1 Installing R packages

There are two methods to installing R packages. Either install them via `yum` or via `CRAN` within R itself. Only a limited number of packages are available via yum so we recommend using R itself.

To find the list of R packages you can install via yum run this command:

```
sudo yum list R-\*
```

Since very few packages are available its best to install packages via CRAN from within R. First start R in a terminal:

```
R
```

then enter the following command:

```
install.packages("pkgname")
```

Replace `pkgname` with the package to install, e.g. for Bio3D:

```
install.packages("bio3D")
```

You can install multiple packages like this:

```
install.packages(c("bio3D","devtools"))
```

The first time you try to install packages R will prompt you to install into your home directory and create a library there, do so and you will be able to install R packages.

Note: If you wish to install the `devtools` package you should first run the command `sudo yum install openssl-devel libcurl-devel libssh2-devel` so that the prerequisite development files are available.

Sadly there is no easy way to allow via `sudo` the ability for you to install R packages system wide so any user can use them. This is because you must first start R as root and execute a specific command. We'll keep working on a way to solve this but as for now you'll need to install R packages in your home directory - sorry about that!

CHAPTER 24

CUDA

CUDA is a mechanism for allowing general purpose computing on graphics cards rather than the normal CPU. It is thus optimised for parallel computing and high memory throughput. CUDA requires a CUDA-enabled graphics processing unit (GPU) which means a NVIDIA graphics card is required.

24.1 Installing CUDA

The NVIDIA CUDA software repository is available on the Linux desktop platform so you can install the various versions like this:

- 8.0: `sudo yum install cuda-8-0`
- 7.5: `sudo yum install cuda-7.5`
- 7.0: `sudo yum install cuda-7-0`

This installs the official NVIDIA CUDA packages. CUDA is installed into:

```
/usr/local/cuda-N.N/
```

Where N.N is the version, e.g. `/usr/local/cuda-8.0`. To add CUDA to your path add this to your `.bashrc`:

```
export PATH=/usr/local/cuda-8.0/bin${PATH:+:${PATH}}
```

24.2 Using CUDA Samples

Once installed you can deploy and build the CUDA samples like this:

```
mkdir ~/cuda
/usr/local/cuda-8.0/bin/cuda-install-samples-8.0.sh ~/cuda
cd ~/cuda/NVIDIA_CUDA*
make
```

That will build *all* the samples, which you probably don't want. Instead change into a sample sub directory and build just one at at time, like so:

```
cd ~/cuda/NVIDIA_CUDA*/0_Simple/clock/
make
```

You can then run the compiled `clock` like so:

```
[db2z07@uos-212247 clock]$ ./clock
CUDA Clock sample
GPU Device 0: "GeForce GTX 750 Ti" with compute capability 5.0

Average clocks/block = 4042.890625
```

CHAPTER 25

OpenMPI

OpenMPI is the defacto standard implementation of the Message Passing Interface system. OpenMPI allows developers to create programs that scale across multiple machines.

25.1 Available versions

Several versions of OpenMPI are available for use:

- Compiled by gcc 4.8
  - 1.10.3 (Red Hat package)
  - 1.10.6
  - 2.0.2
- Compiled by gcc 6.2
  - 1.10.6
  - 2.0.2
  - 2.1.0
- Compiled by icc (Intel)
  - 1.10.6
  - 2.0.2
- Compiled by PGI
  - 1.10.6
  - 2.0.2

The implementations are either compiled with the GNU Compiler Collection (GCC), the Intel C/C++ compiler (icc) or the PGI C/C++ compiler. You can use the implementation and version based on the C/C++ compiler you've chosen to use. All of the GCC versions have been compiled with the RHEL7 default GCC (GCC 4.8). On request we will compile additional versions with newer versions of GCC.

25.2 Installing OpenMPI

Select a version and then run the command for that version listed below. You can install all of the different versions at the same time:

- 1.10.3 (gcc 4.8): `sudo yum install openmpi`
- 1.10.6 (gcc 4.8): `sudo yum install openmpi1106`
- 1.10.6 (gcc 6.2): `sudo yum install openmpi1106-gcc62`
- 1.10.6 (icc): `sudo yum install openmpi1106-intel`
- 1.10.6 (pgi): `sudo yum install openmpi1106-pgi`
- 2.0.2 (gcc 4.8): `sudo yum install openmpi202`
- 2.0.2 (gcc 6.2): `sudo yum install openmpi202-gcc62`
- 2.0.2 (icc): `sudo yum install openmpi202-intel`
- 2.0.2 (pgi): `sudo yum install openmpi202-pgi`
- 2.1.0 (gcc 6.2): `sudo yum install openmpi210-gcc62`

25.3 Using OpenMPI

All of the OpenMPI implementations use the *Environment modules system*. Thus to use an implementation simply `module load` the version you prefer:

- 1.10.3 (gcc 4.8): `module load mpi/openmpi-x86_64`
- 1.10.6 (gcc 4.8): `module load openmpi/1.10.6`
- 1.10.6 (gcc 6.2): `module load openmpi/1.10.6-gcc62`
- 1.10.6 (icc): `module load openmpi/1.10.6-intel`
- 1.10.6 (pgi): `module load openmpi/1.10.6-pgi`
- 2.0.2 (gcc 4.8): `module load openmpi/2.0.2`
- 2.0.2 (gcc 6.2): `module load openmpi/2.0.2-gcc62`
- 2.0.2 (icc): `module load openmpi/2.0.2-intel`
- 2.0.2 (pgi): `module load openmpi/2.0.2-pgi`
- 2.1.0 (gcc 6.2): `module load openmpi/2.1.0-gcc62`

CHAPTER 26

Ruby

Ruby is a dynamic, open source programming language with a focus on simplicity and productivity. According to its developers it it has an elegant syntax that is natural to read and easy to write.

26.1 Installing Ruby

Red Hat Enterprise Linux 7 includes Ruby version 2.0 and can be installed like this in a terminal:

```
sudo yum install ruby rubygems ruby-devel
```

Other versions are also available as part of *SCL*:

- Ruby 1.9.3: `sudo yum install ruby193 ruby193-ruby-devel`
- Ruby 2.2: `sudo yum install rh-ruby22 rh-ruby22-ruby-devel`
- Ruby 2.3: `sudo yum install rh-ruby23 rh-ruby23-ruby-devel`

To use the other versions of Ruby you must first 'enable' them like so:

- Ruby 1.9.3: `scl enable ruby193 bash`
- Ruby 2.2: `scl enable rh-ruby22 bash`
- Ruby 2.3: `scl enable rh-ruby23 bash`

For more information see *Software collections (SCL)*

26.2 Installing gems (packages)

Note: To install Ruby gems via `sudo gem` you need to be in the Administrators group. See *Permissions* for more information. You can also use `gem` without `sudo` to install gems in your home directory.

You can install additional Ruby packages (gems) with the `gem` command line tool:

```
sudo gem install <package>
```

If you're using one of the *SCL* packaged versions of Ruby then you need to run this command instead:

```
sclsudo gem install <package>
```

If you don't have access to run `sudo gem` or you don't want to install the gem for everybody on the system you can install the gem in your home directory instead like this:

```
gem install --user-install <package>
```

To use gems installed in that location you should edit your `~/.bashrc` file and add:

```
if which ruby >/dev/null && which gem >/dev/null; then
    PATH="$(ruby -rubygems -e 'puts Gem.user_dir')/bin:$PATH"
fi
```

And then restart your shell/terminal.

CHAPTER 27

Perl

Perl is an open source dynamic, interpreted general purpose programming language. Perl is primarily a scripting language, but it is also heavily used in web development and bioinformatics.

Perl 5.16 is installed by default on the Linux desktop platform.

27.1 Installing CPAN modules

Note: To install Perl modules via `sudo cpan` you need to be in the Administrators group. See *Permissions* for more information.

You can use sudo to install cpan modules like so:

```
sudo cpan install <modulename>
```

CHAPTER 28

Index of specialist software

28.1 Amber

Assisted Model Building with Energy Refinement (AMBER) is a family of force fields for molecular dynamics of biomolecules originally developed by Peter Kollman's group at the University of California, San Francisco.

- `sudo yum install amber16`

28.2 autodock

AutoDock is a suite of automated docking tools. It is designed to predict how small molecules, such as substrates or drug candidates, bind to a receptor of known 3D structure.

- `sudo yum install autodock426`

28.3 Avogadro

Avogadro is an advanced molecule editor and visualizer designed for cross platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It offers flexible high quality rendering and a powerful plugin architecture.

- `sudo yum install avogadro120`

28.4 BIOVIA Discovery Studio

Built on the BIOVIA Foundation, Discovery Studio is BIOVIA's comprehensive predictive science application for the Life Sciences.

- `sudo yum install biovia-discovery-studio-2016`

28.5 CCDC CSD System

For chemists in academia and industry wanting to discover, access and visualise crystal structures easily to support their research. The CSD-System brings you the essential crystallographic and structural chemistry capabilities to deliver knowledge from the CSD.

- `sudo yum install ccdc2017`

28.6 CUDA

See *CUDA*

28.7 DL_POLY

DL_POLY is a general purpose classical molecular dynamics (MD) simulation software developed at Daresbury Laboratory by I.T. Todorov and W. Smith.

- `sudo yum install dlpoly408`

28.8 Dropbox

Dropbox is the gold standard file hosting and synchronisation solution for modern operating systems. Although we provide this package we offer no support for Dropbox and please do not store any university data within your Dropbox account.

- `sudo yum install nautilus-dropbox`

28.9 FFTW

FFTW is a C subroutine library for computing the Discrete Fourier Transform (DFT) in one or more dimensions, of both real and complex data, and of arbitrary input size.

- `sudo yum install fftw fftw-devel`

28.10 gcc

See *C and C++* and *Fortran*

28.11 GNU Plot

Gnuplot is a command-line driven, interactive function plotting program especially suited for scientific data representation. Gnuplot can be used to plot functions and data points in both two and three dimensions and in many different formats.

- `sudo yum install gnuplot501`

28.12 GROMACS

GROMACS is a versatile package to perform molecular dynamics.

- 4.6.7: `sudo yum install gromacs467`
- 5.1.4: `sudo yum install gromacs514`

28.13 GSView

A user friendly viewer for Postscript, PDF, XPS, EPUB1, CBZ, JPEG and PNG files.

- `sudo yum install gsview60`

28.14 Intel Parallel Studio

See *C and C++* and *Fortran*

28.15 Java

See *Java*

28.16 Kile

Kile is a user friendly (La)TeX source editor and TeX shell.

- `sudo yum install kile`

28.17 LAMMPS

LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator.

- `sudo yum install lammps lammps-doc lammps-openmpi lammps-python`

28.18 latexmk

A make-like utility for LaTeX files. Latexmk is a Perl script for running LaTeX the correct number of times to resolve cross references, etc.

- `sudo yum install latexmk`

28.19 libxc

Libxc is a library of exchange-correlation functionals for density-functional theory. The aim is to provide a portable, well tested and reliable set of exchange and correlation functionals that can be used by all the ETSF codes and also other codes.

- `sudo yum install libxc300`

28.20 LLVM

See *C and C++*

28.21 lyx

LyX is a WYSIYM (What You See Is What You Mean) document editor that acts as a front-end for TeX/LaTeX.

- `sudo yum install lyx`

28.22 Marvin Suite

Marvin Suite is a series of applications and an API for chemical sketching, visualisation and data exploration.

- `sudo yum install Marvin`

28.23 Mathematica

Wolfram Mathematica is a mathematical symbolic computation program, sometimes termed a computer algebra system or program, used in many scientific, engineering, mathematical, and computing fields.

- `sudo yum install mathematica1101`

28.24 MatLab

MATLAB (matrix laboratory) is a multi-paradigm numerical computing environment and fourth-generation programming language.

- `sudo yum install matlab2016b`

28.25 Mendeley Desktop

Mendeley Desktop lets you save PDFs, share thoughts with colleagues and automatically back up and sync your files across different computers.

- `sudo yum install mendeley1178`

28.26 Mercury

Crystal Structure Visualisation, Exploration and Analysis Made Easy. Mercury offers a comprehensive range of tools for 3D structure visualization and the exploration of crystal packing.

- `sudo yum install mercury39`

28.27 MOE

Molecular Operating Environment (MOE) is a drug discovery software platform that integrates visualization, modeling and simulations, as well as methodology development, in one package.

- `sudo yum install moe20160802`

28.28 netcdf

A set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.

- `sudo yum install netcdf`

28.29 NWChem

NWChem aims to provide its users with computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters.

- `sudo yum install nwchem nwchem-openmpi`

28.30 Octave

GNU Octave is a high-level language, primarily intended for numerical computations. It provides a convenient command line interface for solving linear and nonlinear problems numerically, and for performing other numerical experiments using a language that is mostly compatible with Matlab.

- `sudo yum install octave420`

28.31 OpenMPI

See *OpenMPI*

28.32 Perl

See *Perl*

28.33 PGI Compilers

See *C and C++* and *Fortran*

28.34 Povray

The Persistence of Vision Ray Tracer, or PoV-Ray is a ray-tracing program which generates images from a text-based description of a scene.

- `sudo yum install povray37`

28.35 PyMol

PyMOL is a Python-enhanced molecular graphics tool. It excels at 3D visualization of proteins, small molecules, density, surfaces, and trajectories. It also includes molecular editing, ray tracing, and movies.

- `sudo yum install pymol1840`

28.36 Python

See *Python*

28.37 R, RStudio and RStudio Server

See *R*

RStudio is a set of integrated tools designed to help you be more productive with R. It includes a console, syntax-highlighting editor that supports direct code execution, as well as tools for plotting, history, and workspace management.

- `sudo yum install rstudio`
- `sudo yum install rstudio-server`

28.38 SageMath

SageMath is a free open-source mathematics software system licensed under the GPL. It builds on top of many existing open-source packages: NumPy, SciPy, matplotlib, Sympy, Maxima, GAP, FLINT, R and many more.

- `sudo yum install sagemath751`

28.39 Team Viewer

TeamViewer is a proprietary computer software package for remote control, desktop sharing, online meetings, web conferencing and file transfer between computers.

- `sudo yum install teamviewer`

28.40 texlive

See *TeX Live (LaTeX)*

28.41 USCF Chimera

UCSF Chimera is a highly extensible program for interactive visualization and analysis of molecular structures and related data, including density maps, supramolecular assemblies, sequence alignments, docking results, trajectories, and conformational ensembles.

- `sudo yum install chimera1112`

28.42 VirtualBox

VirtualBox is a powerful PC virtualization solution allowing you to run a wide range of PC operating systems on your Linux system. This includes Windows, Linux, FreeBSD, DOS, OpenBSD and others.

- `sudo yum install VirtualBox-5.1`

28.43 VisIT

VisIt is an Open Source, interactive, scalable, visualization, animation and analysis tool.

- `sudo yum install visit2121`

28.44 VMD

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.

- `sudo yum install vmd193`

28.45 VTK

VTK is an open-source software system for image processing, 3D graphics, volume rendering and visualization. VTK includes many advanced algorithms (e.g., surface reconstruction, implicit modeling, decimation) and rendering techniques (e.g., hardware-accelerated volume rendering, LOD control).

- `sudo yum install vtk vtk-qt`

28.46 xdvi

A legacy previewer for DVI files within the X Window System.

- `sudo yum install texlive-xdvi`

28.47 xmgrace

Grace is a WYSIWYG 2D plotting tool for the X Window System and Motif.

- `sudo yum install xmgrace5125`

28.48 xpdf

Xpdf is a legacy viewer for Portable Document Format (PDF) files. Xpdf is a small and efficient program which uses standard X fonts.

- `sudo yum install xpdf`

28.49 Zim Desktop Wiki

Zim is a WYSIWYG text editor written in PyGTK which aims to bring the concept of a wiki to your desktop. Every page is saved as a text file with wiki markup. Pages can contain links to other pages, and are saved automatically.

- `sudo yum install zim`

28.50 Zotero

Zotero is a free, easy-to-use tool to help you collect, organize, cite, and share your research sources.

- `sudo yum install zotero402910`

CHAPTER 29

EPEL

29.1 Extra Packages for Enterprise Linux

EPEL is a repository of extra software packages designed for users of Red Hat Enterprise Linux - the basis of the university Linux desktop platform. EPEL provides a wide range of software packages. EPEL packages are available to install on the university Linux desktop platform and can be installed like any other software package, see *Installing software* for information.

A complete list of EPEL packages is available here.

CHAPTER 30

IUS

30.1 Inline with Upstream Stable

IUS is a repository of add on software for Red Hat Enterprise Linux. It provides up to date copies of important tools like Python, PHP and Git. Although it is intended primarily for use on servers IUS provided packages for Python and PHP offer the latest stable releases and are thus excellent for desktop users of those programming languages too.

A complete list of IUS packages is available here.

CHAPTER 31

RHDT

RHDT, or the Red Hat Developer Toolset, is a bundle of software for developing applications. Bundles are released with new versions once per year and are supported by Red Hat for two years. RHDT uses the *SCL* system so that the tools are installed alongside and do not conflict with the base software within Red Hat Enterprise Linux.

RHDT includes the following packages:

- GCC (C, C++, and Fortran)
- Eclipse IDE
- GDB
- binutils, elfutils
- strace and ltrace
- GNU make
- memstomp
- SystemTap
- valgrind
- Dyninst
- OProfile

CHAPTER 32

SCL

32.1 Software Collections

Sofware collections - or SCL - is a collection of ‘add-on’ software packages created and maintained by Red Hat. They were created in order to deliver more up to date versions of software to customers on Red Hat Enterprise Linux which typically does not update software “mid-life” of a product. Via SCL Red Hat is able to provide more recent stable versions of software for customers to use without affecting the stability and security of the base product.

Due to our education licence all SCL software is available to users of our linux desktops. More information about all the available packages can be found on the dedicated software collections website.