Linux for Biologists

Vimalkumar Velayudhan

Linux for Biologists A Cookbook

Vimalkumar Velayudhan

First edition June 9, 2021



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For Shanthi

Thanks

I would like to express my gratitude to my mentors, colleagues, students, friends and family. Without their support and encouragement, this book wouldn't have been possible.

Thanks also to the wonderful world of Linux and open source software and the community around it.

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About this book

The target audience for this book, what you will need to follow the included recipes and a note on the author.

1.1 Who is it for?

If you are a student or a researcher in biological sciences and are new to Linux, this book will help you get started quickly.

The primary focus is in using graphical user interfaces (GUIs) to accomplish tasks, but I have also included methods using the command line interface.

1.2 What you will learn

Using the included recipes, you will learn how to:

- Run Linux on your computer
- Use the desktop and included software
- Work with files and directories
- Search and install software
- Run some basic commands
- Run the Galaxy platform on your computer

Note: If you need help while following this book...

You can visit the forums of this book on Leanpub. If your query is not answered there, please start a new discussion.

https://community.leanpub.com/c/linuxforbiologi

1.3 What you will need

To follow the recipes in this book, you will need:

- 1. A Linux desktop
- 2. Administrator privileges

1.3.1 Linux desktop

The Linux and open-source world is full of choice.

There are different versions (or distributions) of Linux that are available for download and use.

To ensure that you can follow this book successfully, *Linux Mint* 20.1 is used as a *reference* distribution. All the included recipes have been tested on this distribution.

Virtual machine image

If you do not have access to a Linux desktop, you can download a virtual machine from the website of this book and use it to run a virtual machine on your computer (Fig. 1).



Fig. 1: Linux Mint running in VirtualBox

Follow the steps in *Running a Linux virtual machine* to get started.

What about other Linux distributions?

Although most of the recipes will work on other Linux distributions, you will need to make changes in some cases.

For example, the applications you use might be different — instead of the *Files* file manager used here, you might use Nautilus or Dolphin.

If there are problems, I recommend you download and use the *virtual machine*.

1.3.2 Administrator privileges

The software installation steps in this book will need administrator privileges. In the default configuration, only *root* or members of the sudo user group will be able to install software on a Linux system.

Note: If you are using the *virtual machine*, distributed with this book, you do not need to do anything.

If you are not using the virtual machine, you will need to ensure your user account is part of the sudo group, to be able to install software.

1.4 About the author

Hello. I'm Vimal.

I got introduced to Linux and open source software while pursuing my Master's degree in Biotechnology at Madurai Kamaraj University, India.



The idea of being able to use and modify software without restrictions was new and

exciting to me. I learnt to install Linux, compile software from source code and even create my own Linux live CD!

This experience became valuable in academia, where I worked primarily in research support for a period of over 9 years. During this time, I had installed and managed Linux servers, databases, web applications and websites, contributed in the development of scientific software, published software in repositories, and taught beginner level courses in Python programming and Bioinformatics.

This book is a compilation of the experiences I had gained over time in my interactions with students, colleagues, and the users of our services. Thank you for your interest in reading it. I hope you will find it useful.

Vimalkumar Velayudhan

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Getting started with Linux

In this section, you will learn how to:

- 1. Run Linux on your computer
- 2. Use the desktop and included software
- 3. Work with files and directories
- 4. Start using the command-line and learn some basic commands

2

2.1 Linux — an overview

Linux is an *operating system* developed by Linus Torvalds in 1991. It is released under an open-source licence and the source code is freely available for everyone.

2.1.1 Linux distribution

A Linux distribution includes the Linux operating system with additional software.

Examples: Debian³, Ubuntu⁴, Linux Mint⁵, Fedora⁶, openSUSE⁷ etc.,

³ https://www.debian.org/

⁴ https://ubuntu.com/

⁵ https://linuxmint.com/

⁶ https://getfedora.org/

⁷ https://www.opensuse.org/

2.1.2 Desktop environment

A desktop environment is a *graphical user interface* that provides easy access to files and applications.

Examples:

- GNOME (Fig. 2)
- KDE Plasma (Fig. 3)
- Xfce (Fig. 4)
- MATE (Fig. 5)
- Cinnamon (Fig. 6)

Linux distributions might offer additional variants for download, depending on the desktop environment in use.

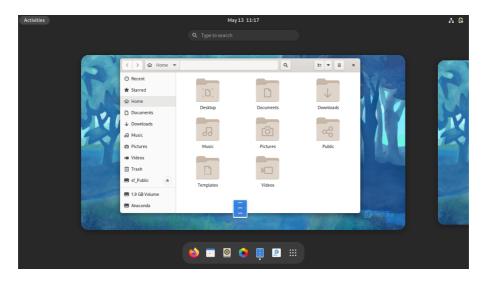


Fig. 2: GNOME

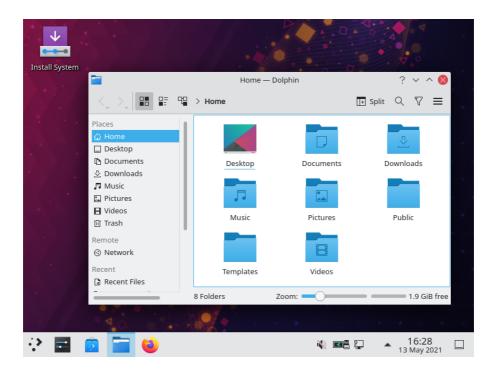


Fig. 3: KDE Plasma

Linux for Biologists

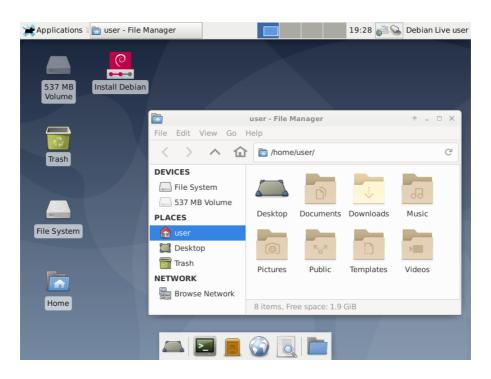
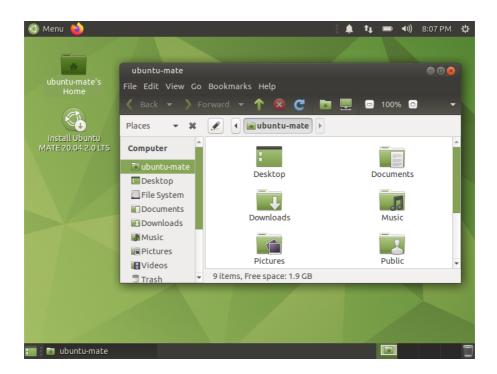
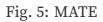


Fig. 4: Xfce





This book uses Linux Mint (Cinnamon)

This book will use Linux Mint 20.1 with the Cinnamon desktop environment as the reference distribution (Fig. 6).

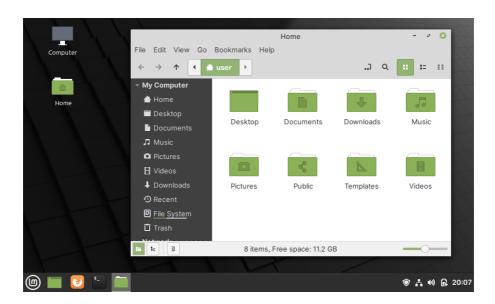


Fig. 6: Linux Mint with Cinnamon desktop environment

All the included recipes have been tested on this distribution.

2.1.3 Ways to run a Linux desktop

To run a Linux desktop on your computer, you can:

- 1. Install a *Linux distribution* or
- 2. Run a virtual machine

I will follow the *second* method in this book, as it is a lot easier for new users to get started.

Note: There are other possibilities, but the methods above are the most common.

2.2 Running a Linux virtual machine

To run virtual machines of other operating systems (guests) on your computer (host), you will need to first install a *hypervisor* software that runs virtual machines.

Examples of hypervisors include VirtualBox, Parallels, VMware Workstation etc., I will use VirtualBox in this book (Fig. 7).

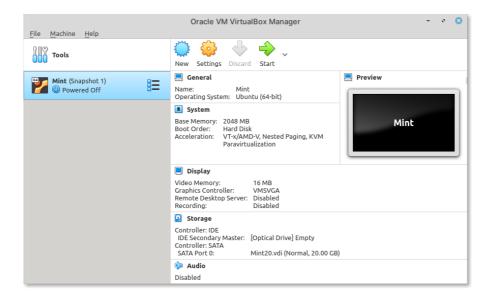


Fig. 7: Main window of VirtualBox

2.2.1 Requirements

VirtualBox installed on your computer

You can install VirtualBox by following the instructions below depending on your operating system.

Attention: Installing software will require administrator privileges.

Instructions for macOS and Windows

You can download an installer for macOS or Windows from the Downloads⁸ section of the VirtualBox website (Fig. 8).

⁸ https://www.virtualbox.org/wiki/Downloads

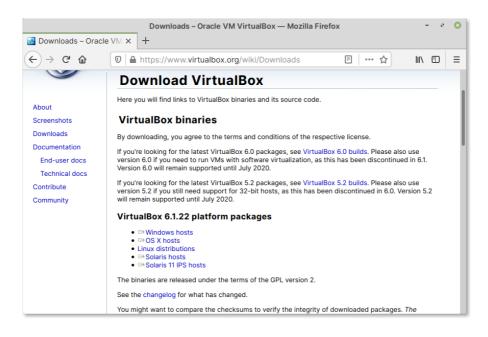


Fig. 8: VirtualBox downloads page

Instructions for Linux distributions

Most Linux distributions include VirtualBox in their package repositories. It is recommended you install it using your package manager like *Synaptic* or *apt*, dnf etc.,

For example, to get VirtualBox working on Ubuntu 20.04 LTS, you will need to install the virtualbox and virtualbox-guest-additions-iso packages.

Note: If you cannot install from repositories, you can download an installer from the Linux Downloads⁹ section of the project

⁹ https://www.virtualbox.org/wiki/Linux_Downloads

website.

Virtual machine image of Linux Mint

You can download a ready-to-use virtual machine image of Linux Mint 20.1 from the website of this book:

https://vimalkvn.com/linuxforbiologists

It is distributed as an *OVA* format file.

Click on the download link and save the linuxmint-20.1.ova file to your computer.

2.2.2 Importing the virtual machine image

Open VirtualBox on your computer and then follow the steps below to import the downloaded virtual machine image.

Step 1 – Select OVA file

From the main window of VirtualBox, select:

```
File \rightarrow Import Appliance (Fig. 9)
```



Fig. 9: Select File -> Import Appliance from the menu

In the Appliance to import screen, click on the button that appears next to the File entry field (Fig. 10).

		Import Virtual Applia	ance							۲
ppliance to im		rt appliance from. This can be	- I I GI b			01/5				
roviders to import clo			a local file syste	m co ir	mport	OVF arc	nive or	one or kno	wn cloud s	ervice
Source: Local File System						\sim				
		virtual appliance from. Virtua ntinue, select the file to impo		upport	s impo	orting ap	pliance	s saved in	the Open	
<u>F</u> ile:										
	F	Please choose a virtual a	ppliance file t	o imp	ort			8		
Look in:	🚞 /home	/user/Downloads	\	←	⇒	↑ D	::::	=		
Comput	er	Name	~	Size		Гуре		Modi		
user		Iinuxmint-20.1.ova		2.40	O GIB	wa File	09/0	5/2		
File <u>n</u> ame:	linuxmint-	20.1.ova					<u>O</u> pe	n Da		
Files of type: Open Virtualization Format (*.ova *.ovf) Cancel										

Fig. 10: Click on the button that appears next to the File entry field

Browse to the location of the linuxmint-20.1.ova file, select it, and then click on the Open button.

The File entry field will now have the complete path to the selected file (Fig. 11).

Ap	ppliance to import	
Pla Pla	lease choose the source to import appliance from. This can be a local file system to import OVF archive or one of known cloud ser roviders to import cloud VM from.	vice
	Source: Local File System	\mathbf{v}
Ple	lease choose a file to import the virtual appliance from. VirtualBox currently supports importing appliances saved in the Open irtualization Format (OVF). To continue, select the file to import below.	
	File: /home/user/Downloads/linuxmint-20.1.ova	
	Expert Mode < Back	A

Fig. 11: Click on the Next button to proceed

Click on the Next button to proceed.

Step 2 — Adjust appliance settings (optional)

In the next screen — Appliance settings (Fig. 12), you can modify the configuration of this virtual machine.

Note: *This step is optional.*

You can click on the Import button at the bottom to proceed to the *next step*.

For example, you can add more CPU or RAM for this virtual machine, depending on the configuration of your computer.

Appliance settings	
These are the virtual machines co change many of the properties sh	ntained in the appliance and the suggested settings of the imported VirtualBox machines. You can own by double-clicking on the items and disable others using the check boxes below.
Virtual System 1	
😓 Name	LinuxMint 20.1
🔒 Guest OS Type	🜠 Ubuntu (64-bit)
CPU	1
RAM	2048 MB
💿 DVD	
Ø USB Controller	
Network Adapter	Intel PRO/1000 MT Desktop (82540EM)
🔷 Storage Controller (IDE)	PIIX4
🔷 Storage Controller (IDE)	PIIX4
🖃 🧇 Storage Controller (SATA)	AHCI
Virtual Disk Image	linuxmint-20.1-disk001.vmdk
🔲 Base Folder	/home/user/VirtualBox VMs
🔂 Primary Group	/
Machine Base Folder: 💼 /home/u	ser/VirtualBox VMs
MAC Address Policy: Include onl	y NAT network adapter MAC addresses
Additional Options: 🔽 Import I	nard drives as VDI
Appliance is not signed	
	Restore Defaults < Back Import Cancel

Fig. 12: Appliance settings screen

Click on the Import button to proceed.

Step 3 — Import progress and completion

You will notice a progress bar at this stage (Fig. 13).

Importing Appliance: Importing appliance '/home/user/Dow						
		'linuxmint-20.1-disk001.vmdk' 44%	(2/3)			
	28 seconds remaining	44 /0	Č			

Fig. 13: Virtual machine import progress

When import is complete, you will be taken back to the main window of VirtualBox.

The imported virtual machine — LinuxMint 20.1, will appear in the panel on the left (Fig. 14).

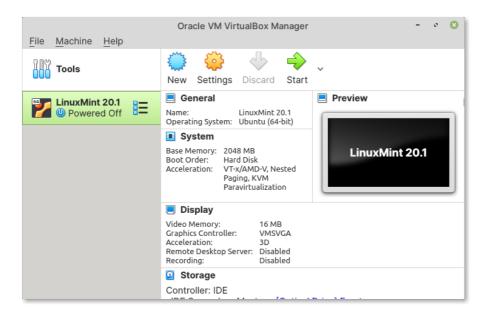


Fig. 14: Imported virtual machine

2.2.3 Starting the virtual machine

To start the virtual machine, select LinuxMint 20.1 and then click on the Start button in the main toolbar (Fig. 15).

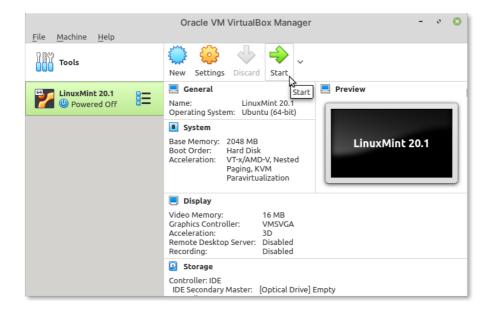


Fig. 15: Start virtual machine

Once the boot process is complete, you will be logged in directly to the desktop (Fig. 16).



Fig. 16: The Linux Mint desktop

For reference, the default username is user and password is also user.

2.2.4 Stopping the virtual machine

When your work is complete, you can shut down the virtual machine by clicking on the Quit button in Linux Mint's Applications Menu.

This will display a confirmation dialog (Fig. 17).

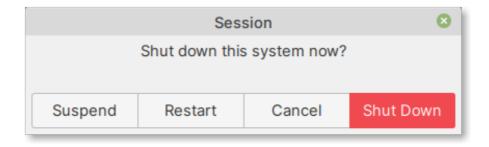


Fig. 17: Confirmation dialog for system shutdown

Click on the Shut Down button to stop the virtual machine.

2.3 The desktop

Once you have started the virtual machine, you will be logged in directly to the desktop.

For reference, the default user account for logging in to the virtual machine, is:

Username: user Password: user

2.3.1 The Cinnamon desktop

In its default configuration, the Cinnamon desktop includes the following components (Fig. 18):

- **Applications Menu** search and launch installed applications, logout, shutdown or restart system.
- **Panel** launch pinned applications, manage open applications windows.
- **System Tray** contains applets for managing the network, sound, power, software updates etc.,

Calendar – provides current date and time, and a calendar.



Fig. 18: Components of the Cinnamon desktop

2.3.2 Changing system settings

The System Settings application can be used to customize the desktop, the operating system and hardware (Fig. 19).

You can launch it from the applications' menu.

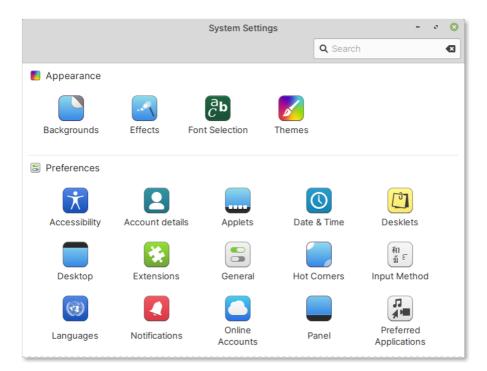


Fig. 19: System Settings application

The settings you can configure here include accessibility, user accounts, date and time, keyboard layout, language, network, display and more.

Changing keyboard layout

The default keyboard layout of the virtual machine is English (US).

You can change this under:

 $Hardware \rightarrow Keyboard \rightarrow Layouts$

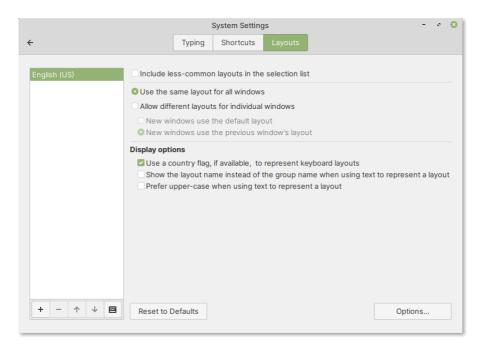


Fig. 20: Keyboard layouts in System Settings

Changing system date and time

The system date and time can be updated by selecting:

 $\mathsf{Preferences} \to \mathsf{Date} \text{ and }\mathsf{Time}$

System Settings	- 0 🖸
÷	
Date and Time	
Region Europe - City Dublin -	
Network time	×
Manually set date and time Monday, 8 March 2021	20:06
Format	
Use 24h clock	
Display the date	×
Display seconds	

Fig. 21: Date and time settings

2.4 Available software

This is a brief overview of applications included in Linux Mint 20.1 Cinnamon.

You can launch them from the Applications Menu (Fig. 22). You can search the list of installed applications using the search bar.



Fig. 22: Launching an application

Note: Some applications discussed here are not included in the default installation.

This includes *GNU Image Manipulation Program* and *Inkscape*. You can install them using *Software Manager*.

2.4.1 Files — manage files and directories

Files is the default file manager (Fig. 23) in Linux Mint.

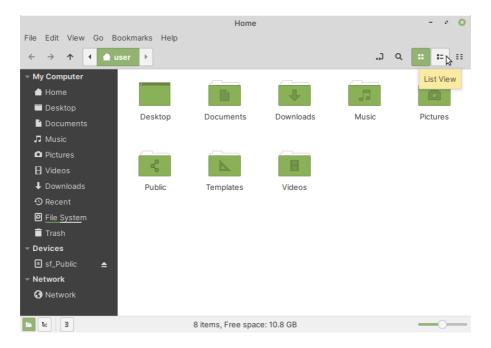


Fig. 23: Main window of Files

Using Files

You can launch Files from the Applications Menu or by clicking on its icon in the Panel.

These are some tips on using Files.

Toggle icon and list views

You can quickly switch between Icon and List View using icons in the toolbar.

Toggle sidebar

You can open the sidebar view or hide it using icons in the status bar.

Open an extra pane

You can open an extra pane using:

View
ightarrow Extra Pane

This is especially useful when you are copying files between local directories or when connected to remote systems.

Bookmark locations

When you are browsing a directory, you can bookmark it if you will access it frequently. This function is available under:

 $\mathsf{Bookmark} \to \mathsf{Add} \; \mathsf{Bookmark}$

Connect to servers

Files can be used to connect to external servers using FTP, SSH, Samba and Webdav. This option is available under:

 $\mathsf{File} \to \mathsf{Connect} \ \mathsf{to} \ \mathsf{Server}$

To learn more about this feature, read the following section in this book: *Transferring files between systems*.

2.4.2 Firefox – browse the web

Firefox is the default web browser (Fig. 24).

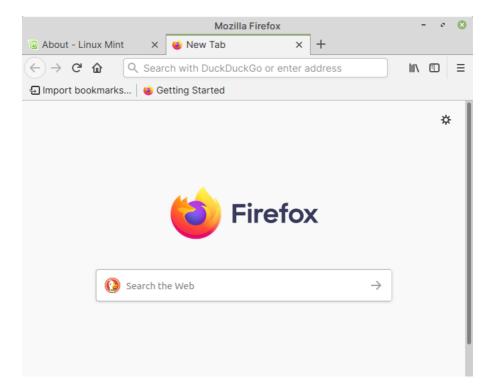


Fig. 24: Firefox web browser

Other web browsers can be installed using *Software Manager*.

2.4.3 Text Editor — create and edit text files

The Text Editor can be used for working with files in plain text formats like .txt, .md and .fasta, or editing configuration files like .bashrc (Fig. 25).

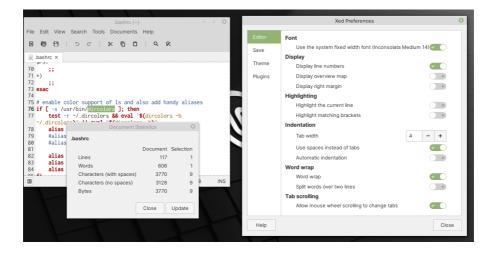


Fig. 25: Text Editor with Document Statistics and Preferences windows open

Using Edit \rightarrow Preferences, you can customize settings like the font used, display of line numbers, indentation, word wrap etc.,

The Tools \rightarrow Document Statistics feature is useful for counting the numbers of words and characters in a document.

Opening hidden files in Text Editor

To open hidden files in Text Editor:

- 1. Use File \rightarrow Open to select a file
- 2. In the Open Files dialog that appears, right-click in the middle pane and select Show Hidden Files (Fig. 26).

	Open Files 📀				
🕙 Recent	🔹 合 user	•			
📥 Home	Name	Open With File Manager	9	Туре	Modified
Desktop	Desktop	Copy Location			17 Feb
Documents	Documents	Add to Bookmarks			Thu
↓ Downloads	Downloads	Show Hidden Files 🔉 🔽			17 Feb
J Music	🔟 Music	Show Size Column			17 Feb
	Pictures	Show Type Column	1		Thu
Pictures	Public	Show Time			17 Feb
🗄 Videos	Templates	Sort Folders before Files 🗧	1		17 Feb
🗂 Trash	Videos				17 Feb
	.bash_histo	bry	190 bytes	Text	Thu
le sf_Public ≜	.bash_logo	ut	220 bytes	Text	17 Feb
+ Other Locations	.bashrc		3.8 kB	Text	17 Feb
	.gtkrc-2.0		22 bytes	Text	17 Feb
	.gtkrc-xfce		516 bytes	Text	17 Feb
Character Encoding:		•			All Files 🔹
				Canc	el Open

Fig. 26: Opening hidden files in Text Editor

You can also use the Ctrl + h keyboard shortcut.

2.4.4 LibreOffice — edit documents and spreadsheets

LibreOffice Writer and LibreOffice Calc can be used to create and edit documents and spreadsheets, respectively (Fig. 27).

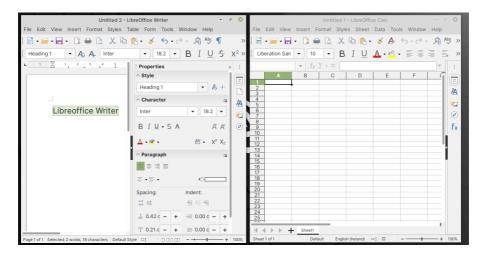


Fig. 27: LibreOffice Writer and Calc programs

The default file formats used by Writer and Calc are ODF Text Document (.odt) and ODF Spreadsheet (.ods) respectively.

These applications also support reading and writing files in Microsoft Office formats like .docx or .doc (Word) and .xlsx or .xls (Excel).

There are additional applications in the LibreOffice suite with functionality to create and edit slide shows or presentations, scientific formulas, diagrams and file-based databases.

2.4.5 Terminal — access the command-line

The Terminal application (Fig. 28) provides the possibility of working with the command-line interface. The default login shell for users on Linux Mint is *Bash*.

	user@cookbook: ~	-	ø	8
File Edit View Search	Terminal Help			
user@cookbook:~\$ ls -1 total 32 drwxr-xr-x 2 user user drwxr-xr-x 2 user user	4096 Feb 17 11:13 Desktop 4096 Feb 17 11:13 Documents 4096 Feb 17 11:13 Downloads 4096 Feb 17 11:13 Music 4096 Mar 3 11:30 Pictures 4096 Feb 17 11:13 Public 4096 Feb 17 11:13 Templates 4096 Feb 17 11:13 Videos			

Fig. 28: Terminal

By selecting the Edit \rightarrow Preferences menu item, you can customize Terminal's appearance and functionality (Fig. 29).

	Preferences – Profile "Unnamed"				
Computer	Global	Text Colors Scrolling Command Compatibility			
		Text and Background Color			
	General	Use colors from system theme			
Home	Shortcuts	Built-in schemes: Solarized dark 🔻			
user@cookbook:~	Profiles +	Text Background Default color:			
File Edit View Search Terminal Help	Unnamed 😔 👻	Bold color:			
user@cookbook:~\$ 1s -1 total 32		Cursor color:			
drwxr-xr-x 2 user user 4096 Feb 17 11:13 Desktop		Highlight color:			
drwxr-xr-x 2 user user 4096 Feb 17 11:13 Documents drwxr-xr-x 2 user user 4096 Feb 17 11:13 Downloads		Use transparent background none full			
drwxr-xr-x 2 user user 4096 Feb 17 11:13 Music drwxr-xr-x 2 user user 4096 Mar 3 11:30 Pictures		Use transparency from system theme			
drwxr-xr-x 2 user user 4096 Feb 17 11:13 Public drwxr-xr-x 2 user user 4096 Feb 17 11:13 Templates		Palette			
drwxr-xr-x 2 user_user 4096 Feb 17 11:13 Videos		Built-in schemes: Solarized -			
user@cookbook:~\$		Color palette:			
		Show bold text in bright colors			
	Help	Close			

Fig. 29: Changing Terminal colour scheme in preferences

2.4.6 Screenshot — take screenshots of desktop or windows

The Screenshot program is useful for taking screenshots of the entire screen, an application window or a selected area of the screen (Fig. 30).

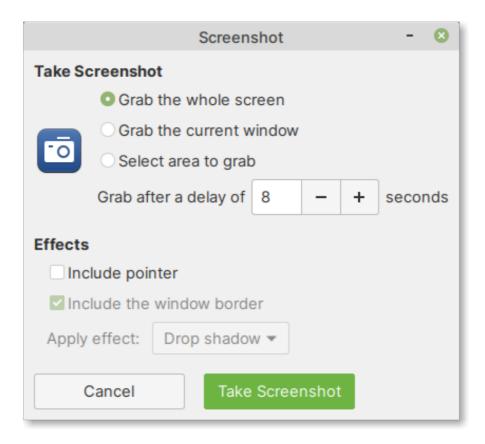


Fig. 30: Screenshot program

2.4.7 Software Manager — install software from repositories

Software Manager can be used to install software from Linux Mint, Ubuntu, Debian and Flathub repositories (Fig. 31).

For a step-by-step procedure for installing software using Software Manager, please consult *The quick and easy method*.

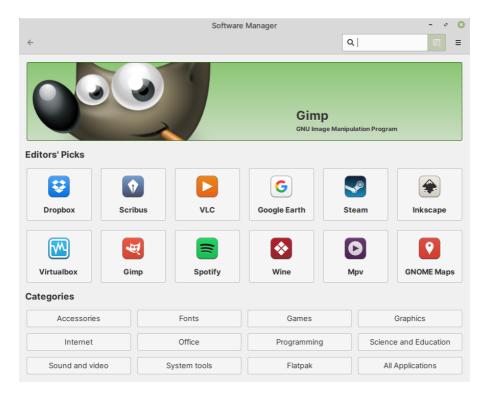


Fig. 31: Software Manager

2.4.8 GNU Image Manipulation Program — edit images

The GIMP program can be used to edit images in various formats like JPG, PNG, TIFF, BMP etc., (Fig. 32).

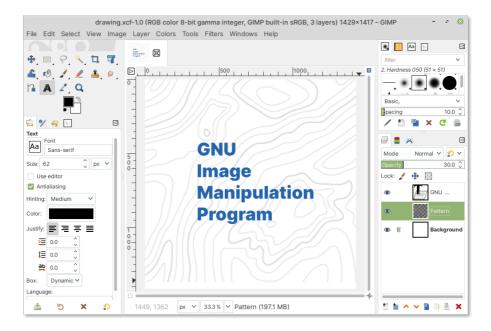


Fig. 32: Editing an image in GIMP

2.4.9 Inkscape - create vector graphics

Inkscape can be used to create and edit images in the scalable vector graphics (SVG) format (Fig. 33).

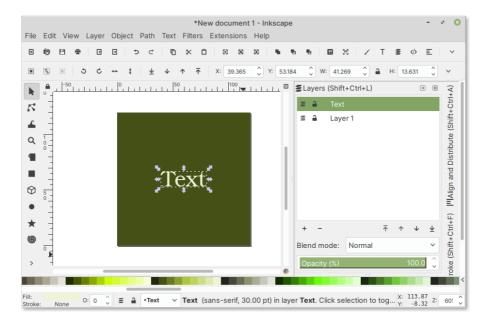


Fig. 33: Creating vector graphics in Inkscape

2.4.10 Notes

Adding an application to favourites

If you use an application frequently, you can consider adding it to favourites. This list is on the left side of the applications' menu.

To favourite an application, right-click on the application name in applications menu and select Add to favorites.

Alternatively, you can choose the Add to panel action, which will add the application to your Panel. Some applications are visible in the Panel by default — a Show Desktop applet, Firefox browser, Terminal, and Files.

Setting default applications

If you would like to set default applications for certain categories or file types, you can do so in System Settings under:

 $\mathsf{Preferences} \to \mathsf{Preferred} \text{ applications}$

2.5 Files and directories

This section includes an introduction to your home directory, files, directories, and their functions, the root filesystem and a how-to on transferring files between systems.

2.5.1 Your home directory

When you log in to the desktop and open *Files*, it will display your home directory (Fig. 34).

The following directories will be present in your home directory by default: Desktop, Documents, Downloads, Music, Pictures, Public, Templates, and Videos.

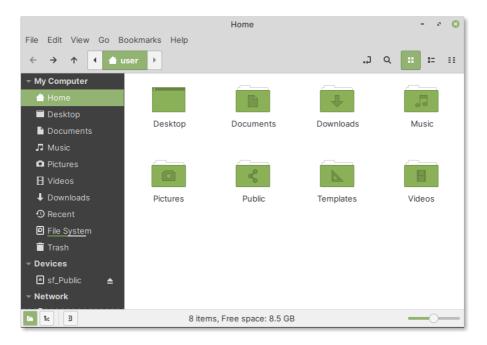


Fig. 34: Home directory

Notes

/home/user

The complete (or absolute) path to your home directory will be of the form /home/user, where user is your username on the system.

\$HOME

The HOME environment variable will automatically be set to the complete path to your home directory in the filesystem.

Hence, you can substitute /home/user with \$HOME in your commands or scripts.

2.5.2 Hidden files and directories

In addition to the default directories mentioned earlier, there are hidden files and directories in home directory (Fig. 35). They have a dot (.) character at the beginning of their file name.

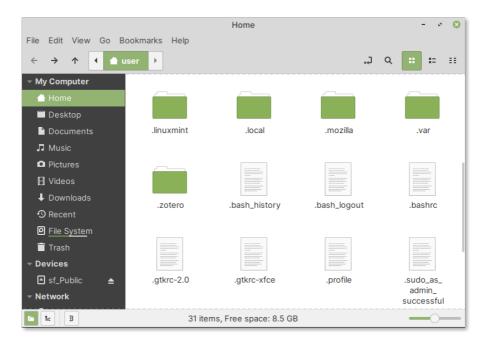


Fig. 35: Hidden files and directories in home directory

You can view (or hide) these files using the following menu entry in file manager:

$\mathrm{View} \to \mathrm{Show}\ \mathrm{Hidden}\ \mathrm{Files}$

Alternatively, you can use the Ctrl + h keyboard shortcut.

2.5.3 Important files in home directory

.bashrc

This is the configuration file used by Bash, the default shell for user accounts. You will mostly use this file, when you need to set or modify environment variables like PATH.

.bash_aliases

You can use the .bash_aliases file to set aliases for commands.

For example, here is a commonly used alias:

```
alias <mark>l='ls -l'</mark>
```

This means when you type l at the command-line, the bash shell will execute ls -l, which will output a long listing of files, instead of the default.

Note: To learn more about the ls command, read the ls - list *files* section.

2.5.4 File and directory names are case-sensitive

One thing you will need to remember is that file and directory names in Linux are case-sensitive.

For example, a file named:

sequence.txt

is different from:

Sequence.txt

Similarly, Documents and documents are two different directories.

Both these files or directories mentioned above, can exist in the same directory and can have different contents.

2.5.5 Accessing the root filesystem

To access the root filesystem (/), click on File System in the sidebar of file manager (Fig. 36).

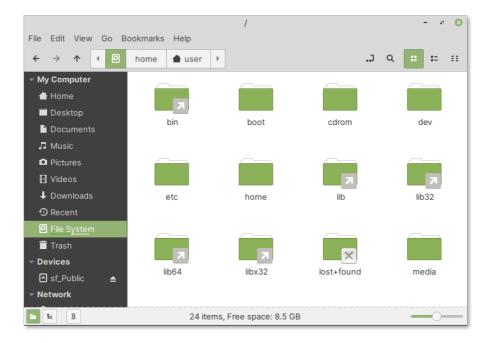


Fig. 36: Click on File System entry to access the root filesystem

Directories under / and their functions

- **/etc** stores configuration files of applications
- **/home** contains home directories of users
- /media locations where devices like external disks will be mounted i.e., made available
- **/root** home directory of root user (administrator)

- /tmp temporary files created by applications
- /usr applications and libraries are installed here along with
 their data and documentation
- /var storage for log files, application cache, databases etc.,

Root file system and root home directory are different

/ is the root filesystem

All users on the system can access files and directories here, provided they have the appropriate permissions.

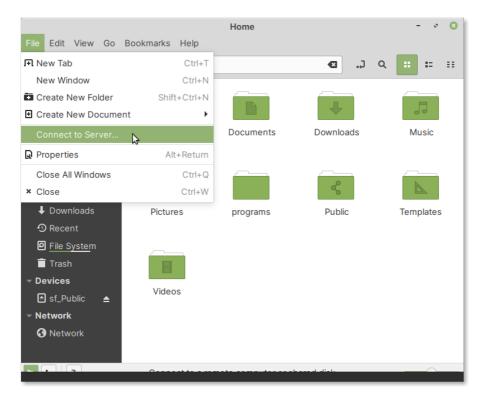
/root is home directory of root

Only root will have access to it.

2.5.6 Transferring files between systems

One useful feature of Files is the ability to connect to remote systems using protocols like SSH, FTP, SMB and Webdav. Once connected, you can transfer files from your Linux desktop to the remote system or *vice-versa*.

To connect to a remote system, use the following menu entry in Files (Fig. 37):



 $\mathsf{File} \to \mathsf{Connect} \ \mathsf{to} \ \mathsf{Server}$

Fig. 37: Connect to Server option in Files

Connecting to an SSH server

Open File \rightarrow Connect to Server and follow the steps below (Fig. 38):

- 1. In the field corresponding to Server, enter the domain name or IP address of the server you are connecting to
- 2. Port 22 is the default for SSH, so you do not need to change that usually
- 3. From the Type drop-down box, select SSH
- 4. Under Folder, you can specify a directory (optional) to open, once connection is successful
- 5. Enter the username and password of your account *on the server*
- 6. Click on the **Connect** button

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		Home	- 0 😣
File Edit View	Go Bookmarks	Help	
$\leftarrow \rightarrow \uparrow$	/home/user) (. 🗈	२ 😐 😐 🖽
- My Computer	_		
📥 Home		Connect to Server	
Desktop	Server Details		
Document	s Server:	server1.example.com Port: 22 - +	Music
J Music	Туре:	SSH 🗸	
Pictures	Folder:	/home/user	
🗄 Videos		home/user	
Downloads	User Details		Templates
🕙 Recent	User name:	user	
File System	Password:	•••••	
Trash		Remember this password	
- Devices		Cancel Connect	
🖻 sf_Public			
- Network			
🚱 Network			

Fig. 38: Connecting to an SSH server

Once the remote directory is open in Files, you can start transferring files from your desktop or *vice-versa*.

Getting software on Linux

In this section, I will discuss how you can get software on your Linux desktop.

For any software you would like to install, you can start with the *quick and easy* method. It will install software available in Linux distribution repositories.

If your software of interest is not available or if you need a different version, you can consider using the other methods.

3.1 The quick and easy method

The *quick and easy* method is to use *Software Manager*, to search and install software on your desktop. It supports installing software from Linux Mint, Debian and Flathub repositories.

Examples of software that can be installed using this method:

 $Circos^{10}$ — plotter for visualizing data.

Clustal Omega¹¹ — general purpose multiple sequence alignment program for nucleotide and protein sequences.

EMBOSS¹² – European molecular biology open software suite.

NCBI BLAST $+^{13}$ — next generation suite of BLAST sequence search tools.

Bioconductor¹⁴ – tools for the analysis and comprehension of high-throughput genomic data.

- **CD-HIT**¹⁵ suite of programs designed to quickly group sequences.
- **UGENE**¹⁶ integrated bioinformatics toolkit.

¹⁰ https://circos.ca

¹¹ https://www.clustal.org/omega

¹² https://emboss.sourceforge.net

¹³ https://blast.ncbi.nlm.nih.gov/Blast.cgi

¹⁴ https://www.bioconductor.org

¹⁵ http://weizhongli-lab.org/cd-hit/

¹⁶ http://ugene.net/

3.1.1 Requirements

Attention: This procedure installs software in system paths and so requires administrator privileges.

3.1.2 Finding and installing software

To demonstrate the steps involved, I will install PyMOL — a software for molecular visualization. You can follow the same procedure for finding and installing other software available in the repositories.

Open Software Manager by clicking on its icon in the applications' menu (Fig. 39).

You can also launch it from the Administration section of the applications' menu.



Fig. 39: Click on Software Manager in applications' menu

When launched, you will see its main window (Fig. 40).

		Software	Manager		- 0	8
÷				٩	R	≡
	3		Firefc Safe and e		vser from Mozilla	
Editors' Picks						
Filezilla	Steam	WhatsApp	Sublime	Scrib		
VLC	Virtualbox	Mpv	Spotify	Chee		
Categories						
Accessories	•	Fonts	Games		Graphics	
Internet		Office	Programming Science and		Science and Education	
Sound and vid	leo	System tools	Flatpak All Applica		All Applications	

Fig. 40: Main window of Software Manager

In the search bar, type pymol.

In some time, packages in repositories that match the search term i.e., pymol, will be displayed below (Fig. 41).

	Software M	Manager	- 0 😣
÷		Q pyn	nol 🛛 🖪 🗏
Pymol Molecular Graphics System	\$		★★★☆☆ 4.7 3 Reviews
Python3-pymol Molecular Graphics System (Python 3 modules)		ជំជំជំជំជំជំ 0 0 Reviews

Fig. 41: Search results for pymol

Click on the first result — Pymol. You will be taken to the package description page.

Note: Why not select Python3-pymol?

The description of the second result, Python3-pymol indicates that it contains Python 3 *modules* for working with PyMOL, which is not what we are looking for.

If you are unsure, you can read the complete description of the package on the next page and confirm if this is the package you

would like to install.

In the package description page, click on the Install button (Fig. 42).

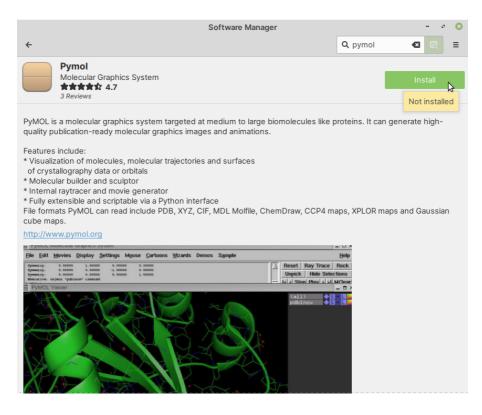


Fig. 42: Click on the Install button to install this package

An dialog window will now appear, prompting you to enter *your password*.

Type in your password and click on the Authenticate button (Fig. 43).

		Software Manager		- 0 0
	< ⊃		Q pymol	
	Pymo Molecu ★★★ 3 Review	ılar Graphics System ★☆ 4.7		Installing
		cular graphics system targeted at medium to large biomole n-ready molecular graphics images and animations.	cules like proteins. It can g	enerate high-
	* Visualiz of crysta	Authenticate		0
	* Molecu * Internal * Fully ex File forma cube mat http://ww File Edit # > Detai	To install or remove software, you need to au An application is attempting to perform an action that re is required to perform this action. Password:		ation
	Byrmet.ry: Byrmet.ry: Breaut.ive: obje		Cancel Authent	icate
			L)	
(1)	1 🕗 🗐 💼	1 💿 📵 🔼 🗝		🄞 🛔 🐠 15:1

Fig. 43: Type in your password and click on the Authenticate button

Installation will now proceed.

When installation is complete, you will notice two buttons — Launch and Remove, in place of the Install button (Fig. 44).

	Software Manager		- 0 😣
÷		Q pymol	
1	Pymol Molecular Graphics System 黄★★★☆ 4.7 3 Reviews	Launch	Remove
Features * Visualiz of crysi * Molecu * Interna * Fully ex	s a molecular graphics system targeted at medium to large biomolecules like publication-ready molecular graphics images and animations. include: cation of molecules, molecular trajectories and surfaces callography data or orbitals lar builder and sculptor I raytracer and movie generator tensible and scriptable via a Python interface ats PyMOL can read include PDB, XYZ, CIF, MDL Molfile, ChemDraw, CCP4 m. ps.	-	-
	vw.pymol.org		
File Edit	Movies Display Settings Mguse Carloons Wizards Demos Sample ○	Help Rock tions	

Fig. 44: Installation complete. Notice the Launch and Remove buttons

Click on the Launch button. This will open the PyMOL program (Fig. 45).

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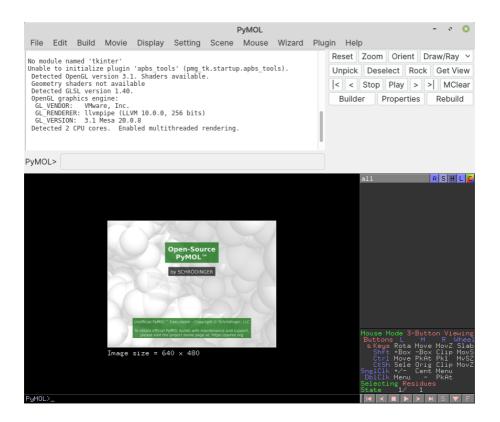


Fig. 45: Main window of PyMOL

Alternatively, you can search for the application in the Applications Menu and launch it from there.

Note: For applications that do not have a graphical user interface, the Launch button will not be present.

If the program includes any commands, you can access them in a *terminal* session.

3.1.3 Removing installed software

You can follow these steps to remove software installed from repositories.

Open Software Manager.

Click on the settings button in the main application window and then select Show installed applications (Fig. 46).



Fig. 46: From Software Manager settings, select Show Installed Applications

Alternatively, you can type the name of the software in the search bar and then press the ENTER key.

In the list of Installed Applications, click on the package you would like to remove — Pymol, in this case (Fig. 47).

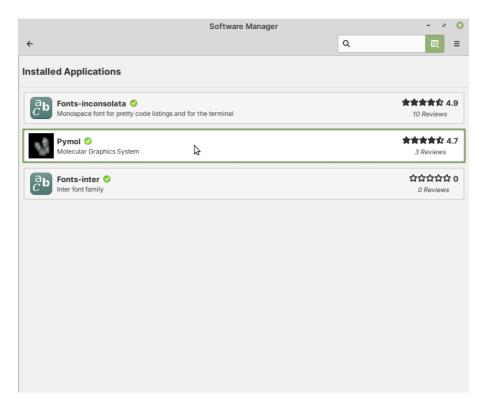


Fig. 47: Click on the package you would like to remove

You will be taken to the package description page.

Click on the Remove button to remove (or uninstall) the package (Fig. 48).

	Software Manager		- • 😣
÷		۹	R
	Pymol Molecular Graphics System ★★★★ 4.7 3 Reviews	Launch	Remove
quality p	s a molecular graphics system targeted at medium to large biomolecules like publication-ready molecular graphics images and animations.	proteins. It can generate	≩ high-
* Visuali of crys * Molecu * Interna * Fully ex	include: ration of molecules, molecular trajectories and surfaces rationy data or orbitals rat builder and sculptor I raytracer and movie generator rtensible and scriptable via a Python interface ats PyMOL can read include PDB, XYZ, CIF, MDL Molfile, ChemDraw, CCP4 m ps.	aps, XPLOR maps and 0	Gaussian
http://ww	vw.pymol.org		
	Movies Display Settings Mouse Cartoons Wizards Demos Sample	Help	
Dynmet.ry: Dynmet.ry: Dynmet.ry:	5 00000 1 00000 5 00000 1.0000 1 00000 1.0000 1 00000 1.0000 1 0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.000	Rock	

Fig. 48: Click on the Remove button to remove the package

You will be prompted to enter your password.

Type in *your password* and then click on the Authenticate button to proceed (Fig. 49).

				Softwa	ire Manager				- 0 🛞	
	< υ →						۹		₽ =	
	Pymol Molecular ★★★★ 3 Reviews	Graphics Sys 4.7	stem					Remo	ving	
	PyMOL is a molecula publication-ready mo					cules like prote	eins. It can	generate hig	Jh-quality	
	* Visualizat of crystall			Auti	nenticate			0	1	
	* Molecula * Internal ra * Fully exte File format: maps. http://www Bie Eat More	An applicati is required Password:		ing to perform is action.	you need to a				sian cube	ł
	Rywwelry: 0. Sywwelry: 0. Sywwelry: 0. Brecutive: cejmot					Cancel	Auti	nenticate		
	PAAC Walk					LLI)	>			
(1)	🛛 🔁 🖿	💿 🔼	🔲 🗝	>					A 🔊	•0) 15:3

Fig. 49: Type in your password and click on the Authenticate button

The software will now be removed (or uninstalled) from the system.

3.1.4 Updating installed software

When updates are available for software installed on your system, you will see a notification in the system tray (Fig. 50).



Fig. 50: Notification of software updates in system tray

To apply software updates:

Click on the notification icon in system tray. This will open the Update Manager program.

To install all available software updates, click on the Install Updates button in the toolbar (Fig. 51).

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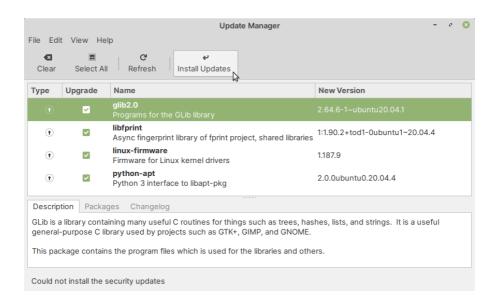


Fig. 51: Click on the Install Updates button to apply all available updates

You will be prompted to enter your password (Fig. 52).

Type in *your password* and click on the Authenticate button.

Clear Select		New Version	
•	glib2.0 Programs for the GLib library	2.64.6-1~ubuntu20.04.	1
(†)		enticate	0
 (†) (†) 	Synaptic An application is attempting to perform is required to perform this action. Password:	an action that requires privileges. Auther	ntication
Description GLib is a libra general-purp	etails	Cancel	enticate
his package con	tains the program files which is used for the l	libraries and others.	
Installing updates			

Fig. 52: Type in your password and click on the Authenticate button

Update Manager will now continue installing updates (Fig. 53).

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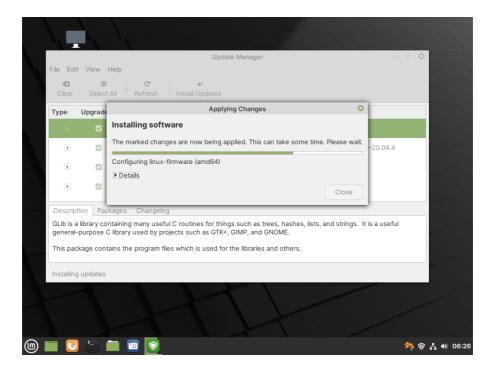


Fig. 53: Update Manager installing software updates

When the update process is complete, you will see a message — Your system is up to date (Fig. 54).

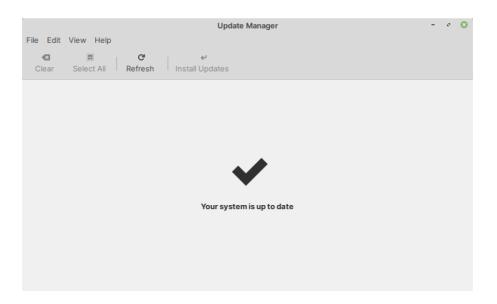


Fig. 54: Updates installed successfully

3.1.5 Notes

The command-line version (apt)

You can use the *apt* package manager to install software from the command-line.

Searching for software

Open a terminal to perform a search for matching packages in the repositories.

For example, here is a search for pymol

apt search pymol

Note: You do not need to include sudo here.

This will output matching results from repositories, if any:

р	pymol	- Molecular Graphics System
р	pymol-data	- data files for PyMOL
р	python3-pymol	- Molecular Graphics System (Python 3
⊶m	odule	

Once you have identified the correct package name — in this case, it is pymol you can proceed towards installing the package.

Installing a package

You can install a package using the following command:

```
sudo apt install pymol
```

Attention: You need to include sudo here.

Also, in the commands below, you will be asked to enter *your password*.

You will also need to confirm if you would like to continue with the changes. Type y and then press the ENTER key to proceed.

```
[sudo] password for user:
Reading package lists... Done
Building dependency tree
Reading state information... Done
The following additional packages will be installed:
    pymol-data python3-pymol
The following NEW packages will be installed:
    pymol pymol-data python3-pymol
0 upgraded, 3 newly installed, 0 to remove and
4 not upgraded.
Need to get 0 B/5,192 kB of archives.
After this operation, 19.8 MB of additional disk
space will be used.
Do you want to continue? [Y/n] y
```

The package will now be installed.

Removing an installed package

To remove an installed package, use the command:

sudo apt remove pymol

The command above does not remove dependent packages. You can remove them using:

sudo apt autoremove

Updating packages

To update *all installed packages*, you can use these commands:

sudo apt update sudo apt upgrade

To update *a specific package* — if an update is available, you can simply use apt install again:

sudo apt install package_name

Why is this a quick and easy method?

You can use a graphical user interface (Software Manager) or the command-line (apt) to install software available in Linux package repositories.

Software installed in this manner will also be kept updated along with the rest of the system.

Additional software repositories

It takes some time for newer versions of software to become available in distribution repositories.

If your software of interest is not available or if you need a more recent version of the software, you could try installing them from these additional sources:

- Python packages from PyPI
- Perl modules from CPAN
- R packages from CRAN or Bioconductor
- Conda packages from Anaconda Cloud

Attention: Software installed using these methods, will also need to be kept updated manually.

3.2 Python packages

If your software of interest is available as a Python package on PyPI, you can install it using pip — Python package installer.

Note: Your software might already be available using *The quick and easy method*. Search for package names starting with python-.

In certain cases, installing packages in a virtual environment might be a better option. Read:

-> When should I use a virtual environment?

3.2.1 Requirements

Python package installer (pip)

To install pip, follow *The quick and easy method* for installing software.

Search and install the python3-pip package.

\$HOME/.local/bin added to \$PATH

Packages that include commands will install them in the \$HOME/.local/bin directory (*What is \$HOME?*).

To be able to run these commands easily, you will need to add this directory to your \$PATH variable. You can do so by following the steps in *Adding directories to PATH*.

Attention: You should not add sudo in the commands below.

This method only installs files in your home directory and so does not require administrator privileges.

3.2.2 Searching for a package on PyPI

Open PyPI website¹⁷ in a web browser.

In the Search projects field, enter the name of the software you would like to install and press the ENTER key or click on the search button (Fig. 55).

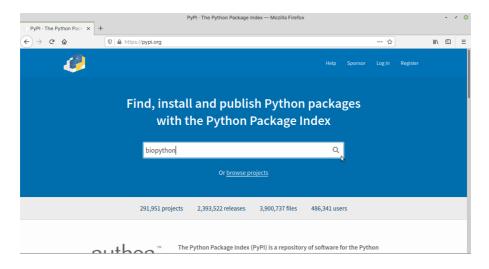


Fig. 55: Searching for a package on PyPI

A list of packages matching the search term will be displayed (Fig. 56).

¹⁷ https://pypi.org

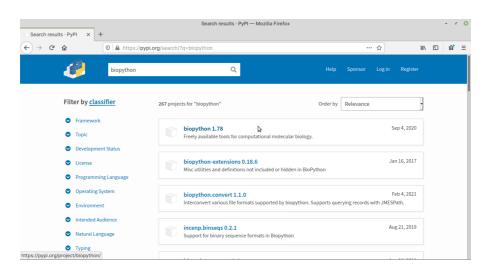


Fig. 56: Search results for biopython. 1.78 is the version number.

Click on the result to proceed to the project description page.

In the project description page, find the package name (Fig. 57) in the pip install command.

In this case, it is biopython.

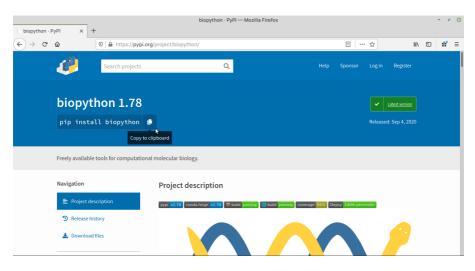


Fig. 57: Project description page for Biopython

Note: You will need to use pip3 instead of the pip command in the steps below. *Why?*

You can now proceed towards installing the package.

3.2.3 Installing a Python package

Open a terminal.

Use the pip3 install command with by the name of the package, you would like to install.

Using biopython as an example:

pip3 install biopython

Output:

Note: One limitation of this method is that, you will not be able to install *multiple versions* of a package. This can be solved using a *virtual environment*.

3.2.4 Updating an installed package

When you notice an update is available for the package, you can use the install command with the -U option, and the name of the package:

```
pip3 install -U biopython
```

3.2.5 Removing an installed package

Use the uninstall command with the name of the package you would like to remove:

pip3 uninstall biopython

3.2.6 Using installed packages

Where are the files installed?

You can use the pip3 show command with the name of the package to identify the path where it is installed:

pip3 show biopython

Output:

Name: biopython Version: 1.78 Summary: Freely available tools for computational →molecular biology. Home-page: https://biopython.org/ Author: The Biopython Contributors Author-email: biopython@biopython.org License: UNKNOWN Location: /home/user/.local/lib/python3.8/site-packages Requires: numpy Required-by:

The installation path will be listed next to the Location keyword.

Using Python packages and modules

Python packages and modules will be installed in \$HOME/. local/lib/python3.8/site-packages.

Note: This is the path for Python 3.8.

If you have a different version of Python installed, this value will change.

This directory will be automatically included in \$PYTHONPATH. So, you can import and use installed packages and modules in your scripts, without any extra effort.

For example, here is a simple Python script to test BioPython installed using pip:

```
from Bio.Seq import Seq
seq = Seq('ATGC')
comp = seq.complement()
print(f'The complement of {seq} is {comp}')
```

The Bio.Seq package is part of BioPython. Copy the code sample above and save it as biopy_test.py. Then run it from the terminal like so:

python3 biopy_test.py

Output:

The complement of ATGC is TACG

Using included commands

If the package includes commands, those will be installed in \$HOME/.local/bin directory. For these commands to be easily accessible, you will need to add this directory to PATH, as mentioned under *requirements*.

As an example, when you install the Python package of *cutadapt*, the cutadapt command will be installed in \$HOME/.local/bin, which you can then run from a terminal like this:

```
cutadapt --version
```

Output:

3.1

3.2.7 Python virtual environments

A virtual environment is a *self-contained* directory tree containing Python and some additional packages.

Advantages

These are *some* advantages of using virtual environments.

No administrator privileges

You do not need administrator privileges to create a virtual environment or install packages in an environment.

Multiple environments

Multiple virtual environments can be created with each containing their own sets of packages.

These are isolated and packages in an environment can be installed, updated or removed without affecting other environments.

Share your environment

You can share your configuration with others. They will be able to reproduce your environment, with the exact versions of packages.

Creating a virtual environment

First, using *The quick and easy method*, search and install the python3-venv package. This includes the venv module necessary for creating virtual environments.

You can create a virtual environment in any directory where you have write privileges, for example, your home directory.

To demonstrate, I will create a virtual environment called py3env in my home directory.

```
python3 -m venv py3env
```

If successful, you will find a directory named py3env in the current directory. No messages will be displayed.

Note: python3 is the command to run the Python 3 interpreter. Its complete path is /usr/bin/python3.

venv is the Python module to create virtual environments.

The -m option runs the venv module as a script.

Before you can use a virtual environment, you will need to activate it.

Activating a virtual environment

You will need to activate a virtual environment before you can start using it. To do so, use the source command with the path to the virtual environment's activate script.

For example, to activate py3env created in the *previous step*, use:

```
source py3env/bin/activate
```

Your shell prompt will now change to indicate that the virtual environment is now active. Note the (py3env) label at the beginning of the prompt:

```
(py3env) user@cookbook:~$
```

You can now start using this virtual environment.

Note: Before you start installing packages...

It is a good idea to install (or upgrade) Python build tools – *pip*, *setuptools*, and *wheel* in a new virtual environment.

These build tools are necessary for building and installing packages from *PyPI* and other sources.

Installing them will ensure that additional packages will build and install without errors.

Installing Python build tools

Use pip3 install to install or upgrade the required packages:

pip3 install -U pip setuptools wheel

The -U option of pip3 install, will upgrade listed packages, if newer versions are available.

Output:

```
Collecting pip
Downloading pip-21.0.1-py3-none-any.whl (1.5 MB)
...
Installing collected packages: pip, setuptools, wheel
...
Successfully installed pip-21.0.1 setuptools-54.2.0 wheel-
→0.36.2
```

Deactivating a virtual environment

To exit a virtual environment, use the command:

deactivate

Your shell prompt will change to its original appearance:

user@cookbook:~\$

3.2.8 Notes

You will need to update these packages manually

Packages installed in this manner should also be updated manually.

When you notice there is an update for the package, for example, from the project's website or from their source code repository, follow the steps in *Updating an installed package* to install the latest version.

Why pip3 and not pip?

The *pip* package includes the following commands:

- pip3 Python 3 version
- pip Python 2 version

Support for Python 2 ended in January 2020.

Since there is a possibility for both commands to exist on a system, it is safer to use pip3 when installing packages using this method.

What about programs written in Python 2?

Support for Python 2 ended in January 2020.

If you do need to use a program written only in Python 2, you can create an isolated environment — either using Python venv or Conda and then install the package there.

Related sections:

- Python virtual environments
- Conda packages

When should I use a virtual environment?

The method described here will not work if the programs you are installing require two different versions of the same package from PyPI.

In that case, you can consider creating an isolated environment — either using Python virtualenv or Conda and then installing the packages there.

Related sections:

- Python virtual environments
- Conda packages

Older versions of pip

If the version of pip installed in your system is older than 20.0, it will attempt to install packages in system paths by default, resulting in *permission denied* errors.

To avoid that, you will need to add the --user option to the install and uninstall commands, for example:

```
pip3 install --user biopython
```

A better approach is to *upgrade* your local version of pip. Once upgraded, you will no longer need to user --user.

To upgrade pip, do:

pip3 install --user -U pip

You can check the installed version of pip using:

pip3 -V

3.3 Perl modules

For installing Perl modules, you can configure the *local-lib* module to create and use a local directory. The default location is \$HOME/perl5.

If your software of interest is available on *CPAN*, you can install it easily using the *cpanminus* script.

Note: Your software of interest, might be available using *The quick and easy method*.

Search for package names containing perl.

3.3.1 Requirements

The build-essential and cpanminus packages installed

If you do not have them installed, follow *The quick and easy method*, and search and install the following packages:

- build-essential installs compilers and build tools like make
- 2. **cpanminus** script to obtain, build and install modules from CPAN along with their *dependencies*

Attention: You should not add sudo in the commands below.

This method only installs files in your home directory and so does not require administrator privileges.

3.3.2 Configuring local-lib module

To configure local-lib:

Open the \$HOME/.bashrc file in a *text editor*.

Add the following text at the end of the file:

Configuration for Perl local-lib module
eval "\$(perl -Mlocal::lib)"

Save the file.

Here is a sample .bashrc, for reference (Fig. 58).

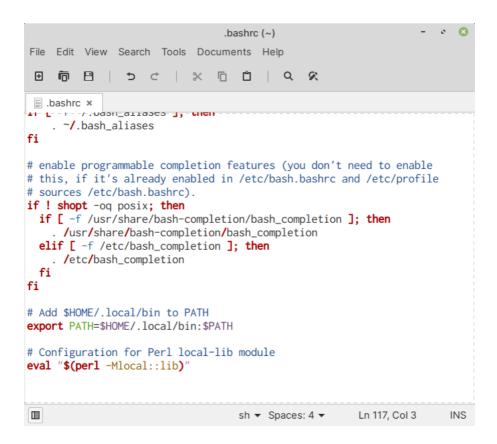


Fig. 58: local-lib configuration in .bashrc

Open a new terminal window.

You will notice the following message displayed (Fig. 59):

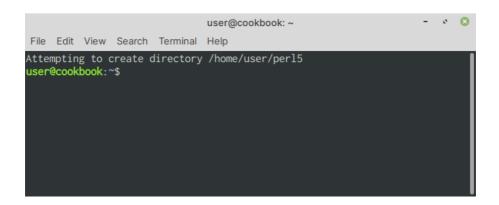


Fig. 59: Attempting to create directory /home/user/perl5

Configuration is now complete.

You can now start installing modules from CPAN and other sources.

3.3.3 Searching for a module on CPAN

Open *MetaCPAN* website (https://metacpan.org) in a web browser.

In the Search field, enter the name of the module you would like to install and click on the Search the CPAN button.

I will use David H. Ardell's *FAST* package as an example. (Fig. 60).

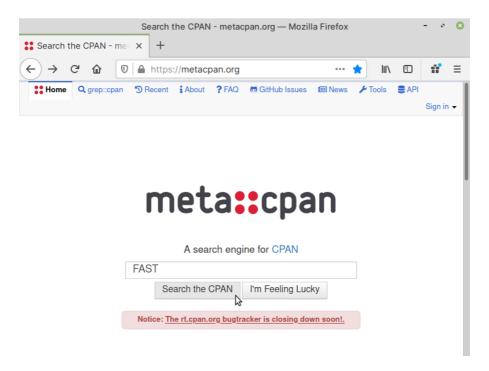


Fig. 60: Searching for a module on MetaCPAN

This should display modules matching the search term — FAST (Fig. 61).

Linux for Biologists

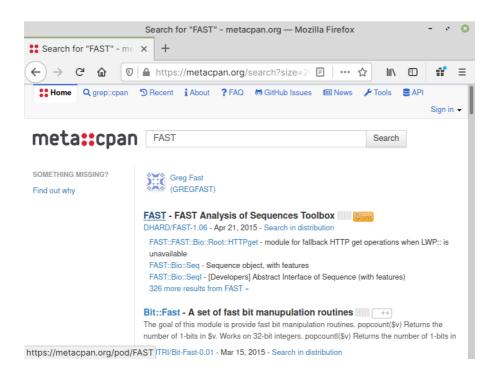


Fig. 61: Search results for modules

If you click on the *appropriate* module name, you will be taken to a description page, where you can learn more about the module (Fig. 62).

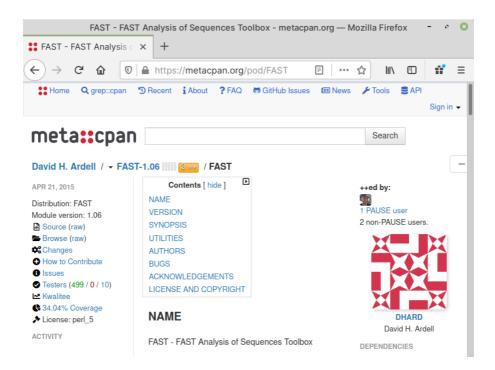


Fig. 62: Module description page

On this page, you can also verify the module name to use in the next step.

To do that, click on Install Instructions under TOOLS menu in the sidebar. This will open a pop-up window with information on the module name you need to use with the cpanm command.

In this case, the module name to use, is simply called FAST (Fig. 63).

Linux for Biologists

	FAST - FAST Analysis of Sequences Toolbox - metacpan.org — Mozilla Firefox	-	e 😣
FA	ST - FAST Analysis ⊂ × +		
€	→ C l l https://metacpan.org/pod/FAST 🗉 🗠 🟠 💷	D n	! ≡
Dis Mc	Module Install Instructions	×	
000	To install FAST, copy and paste the appropriate command in to your terminal.		
12 13 14	cpanm FAST		
AC	CPAN shell		
то	perl -MCPAN -e shell install FAST		
	For more information on module installation, please visit the detailed CPAN module installation guide	э.	
>_		Close	

Fig. 63: Module install instructions for FAST

You can now proceed towards installing this module.

3.3.4 Installing a Perl module

Open a terminal window.

Install the module with the cpanm command:

cpanm FAST

This will install the module and its dependencies, if there are any.

Output:

```
--> Working on FAST
Fetching http://www.cpan.org/authors/id/D/DH/DHARD/FAST-1.
→06.tar.gz ... 0K
Configuring FAST-1.06 ... 0K
=> Found dependencies: Bit::Vector, Sort::MergeSort,
→Sort::Key
--> Working on Bit::Vector
Fetching http://www.cpan.org/authors/id/S/ST/STBEY/Bit-
→Vector-7.4.tar.gz ... 0K
Configuring Bit-Vector-7.4 ... 0K
...
Building and testing FAST-1.06 ... 0K
Successfully installed FAST-1.06
6 distributions installed
```

3.3.5 Using installed modules

Using included commands

If the module includes commands, those will be installed in \$HOME/perl5/bin. This directory will be included in \$PATH, when you *configured* local-lib. Hence, you can start using the commands included in a module immediately after installation.

For example, here is the help page of the fasuniq command included with the FAST package installed in the previous step:

```
fasuniq -h
Usage:
   fasuniq [options] [MULTIFASTA-FILE]
   [MULTIFASTA-DATA-ON-STDIN] | fasuniq [options]
...
```

Using modules in your scripts

Modules will be installed in:

```
$HOME/per15/lib/per15/5.30.0.
```

Note: This is the module path for Perl 5.30.0.

It you have a different version of Perl installed on your system, it will change.

As local-lib makes these modules discoverable automatically, you can start using them in your scripts immediately.

Here is an example using the *Bio::Phylo* package. After installing the module with cpanm Bio::Phylo, create a file using a text editor and copy the following content:

```
use Bio::Phylo;
```

print version
print Bio::Phylo->VERSION;

print citation
print Bio::Phylo->CITATION;

Save the file as biophylo_test.pl and then run it:

```
perl biophylo_test.pl
```

Output:

```
v2.0.1Rutger A Vos, Jason Caravas, Klaas Hartmann, Mark A

→Jensen and Chase Miller, 2011.

Bio::Phylo - phyloinformatic analysis using Perl. BMC

→Bioinformatics 12:63.

doi:10.1186/1471-2105-12-63
```

3.4 R packages

If your software of interest is available as an R package on *CRAN* or *Bioconductor*, you can install it using the install.packages() or BiocManager::install() commands respectively.

Note: Your software might already be available using *The quick and easy method*.

Search for package names starting with r-cran- or r-bioc-.

3.4.1 Requirements

The r-base package installed

The **r**-base package provides the GNUR statistical computation and graphics system.

If you do not have it installed, follow *The quick and easy method*, and search and install the r-base package.

Attention: You should not add sudo in the commands below.

This method only installs files in your home directory and so does not require administrator privileges.

3.4.2 Starting an R session

To start an R session, open a terminal window.

Type the R command and press the ENTER key.

```
user@cookbook:~$ R
```

You will be placed inside an R session. Some additional information will be displayed, including the version of R installed.

You can type R commands at the > prompt.

```
R version 3.6.3 (2020-02-29) -- "Holding the Windsock"
Copyright (C) 2020 The R Foundation for Statistical

Gomputing

Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.

You are welcome to redistribute it under certain

Gonditions.

Type 'license()' or 'licence()' for distribution details.

Natural language support but running in an English

Gocale

R is a collaborative project with many contributors.

Type 'contributors()' for more information and
```

'citation()' on how to cite R or R packages in →publications.

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```
Type 'demo()' for some demos, 'help()' for on-line help,⊠

→or

'help.start()' for an HTML browser interface to help.

Type 'q()' to quit R.
```

>

3.4.3 Installing a package from CRAN

You can search for R packages on CRAN by consulting the Task Views¹⁸ for a categorized listing or the Table of available packages¹⁹ (currently 17157 packages). Once you have identified a package to install, you can follow the steps below to install it.

I will install the *BiocManager* package as an example below.

1. Install package using install.packages() command

Start an R session.

At the prompt, type the install.packages() command with the name of the package in quotes. For example:

install.packages("BiocManager")

Press the ENTER key to proceed.

2. Confirm use of personal library

You will notice a prompt requesting you to confirm if you would like to use a personal library:

```
Installing package into '/usr/local/lib/R/site-library'
(as 'lib' is unspecified)
```

(continues on next page)

```
<sup>18</sup> https://cran.r-project.org/web/views/
```

¹⁹ https://cran.r-project.org/web/packages/available_packages_by_name. html

(continued from previous page)

```
Warning in install.packages("BiocManager") :
'lib = "/usr/local/lib/R/site-library"' is not writable
Would you like to use a personal library instead? (yes/No/
→cancel) yes
```

Type yes to confirm and press the ENTER key. *Why use a personal library*?.

3. Create personal library if necessary

If you have never installed a package, the personal library directory will not exist. If so, you will be prompted for confirmation to create it:

```
Would you like to create a personal library
'~/R/x86_64-pc-linux-gnu-library/3.6'
to install packages into? (yes/No/cancel) yes
```

Type yes to confirm and press the ENTER key.

Note: The next time you install a package, you will not see this prompt.

4. Package installation summary

Installation should now proceed:

```
trying URL 'https://cloud.r-project.org/src/contrib/
→BiocManager_1.30.10.tar.gz'
Content type 'application/x-gzip' length 40205 bytes (391
→KB)
downloaded 39 KB
* installing *source* package 'BiocManager' ...
** package 'BiocManager' successfully unpacked and MD5
→sums checked
** using staged installation
** R
** inst
** byte-compile and prepare package for lazy loading
** help
*** installing help indices
** building package indices
** installing vignettes
** testing if installed package can be loaded from
→temporary location
** testing if installed package can be loaded from final
→location
** testing if installed package keeps a record of
→temporary installation path
* DONE (BiocManager)
```

(continues on next page)

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```
The downloaded source packages are in
    '/tmp/RtmpDgm0Z8/downloaded_packages'
>
```

If there are no errors during the process, the package installation is successful.

3.4.4 Installing a package from Bioconductor

You can search the Bioconductor software package list²⁰ on the website (currently has 1974 packages). Once you have identified a package to install, you can follow the steps below to install it.

I will install the *edgeR* package as an example.

Install package using BiocManager::install() command

- 1. Start an R session.
- 2. *Install the BiocManager package*. This is necessary for installing R packages from Bioconductor repository.

Note: You only need to do this once.

The next time you wish to install a package from Bioconductor, you can proceed to step 3.

 At the R prompt, use the BiocManager::install() command with the name of the package you would like to install in quotes.

For example:

```
BiocManager::install("edgeR")
```

Press the ENTER key to proceed.

²⁰ https://www.bioconductor.org/packages/release/BiocViews.html#__ _Software

The package and its dependencies will now be down-loaded, compiled and installed.

Output:

```
Bioconductor version 3.10 (BiocManager 1.30.10), R 3.

→6.3 (2020-02-29)

Installing package(s) 'BiocVersion', 'edgeR'

also installing the dependencies 'limma', 'locfit',

→ 'Rcpp'

....

** testing if installed package can be loaded from

→ temporary location

** checking absolute paths in shared objects and

→ dynamic libraries

** testing if installed package can be loaded from

→ final location

** testing if installed package keeps a record of

→ temporary installation path

* DONE (edgeR)
```

If there are no errors during the process, the package installation is successful.

3.4.5 Updating an R package

When an update is available for a package, use the following commands to update.

For packages installed from CRAN:

```
install.packages("BiocManager")
```

For packages installed from Bioconductor:

```
BiocManager::install("edgeR")
```

3.4.6 Removing an R package

To remove an installed package, use the remove.packages() command with the name of the package in quotes.

For example:

```
remove.packages("BiocManager")
```

3.4.7 Notes

The r-base-dev and build-essential packages

If you are installing additional packages from CRAN and other sources, you will also need to install the r-base-dev and build-essential packages. However, when you install r-base, these packages will also be installed as dependencies so, you do not have to install them manually.

Why use a personal library?

When installing packages, R will first attempt to use a system library — for example, /usr/local/lib/R/site-library. This path can only be modified by a user with administrator privileges. This is why a personal library in the \$HOME directory is a better option for users to install packages.

3.5 Conda packages

You can use the *Conda* package manager to create isolated environments and install software available from *Anaconda Cloud* repositories.

These environments can be activated, deactivated and removed when they are no longer needed.

3.5.1 Requirements

Attention: You should not add sudo in the commands below.

This method only installs files in your home directory and so does not require administrator privileges.

3.5.2 Installing Conda

A minimal installation of Conda can be setup by installing *Miniconda*. You will need to download and run the Miniconda installer following the steps below.

1. Downloading Miniconda

To download the correct version of Miniconda:

- 1. Open the Conda downloads²¹ page in a browser.
- 2. Navigate to the Linux installers section (Fig. 64)

🕷 Conda latest	Linux insta	llers		
Search docs				Linux
Conda	Python version	Name	Size	SHA256 hash
Conda-build	Python 3.8	Miniconda3 Linux 64-bit	88.7 MiB	879457af6a8bf5b34b48c12de31d4df8ee2f86a8e68768e5758c3293b2daf688
∃ Miniconda	Python 3.7	Miniconda3 Linux 32-bit	62.7 MiB	f387eded3fa4ddc3104b7775e62d59865b38285c2758a8b86b4c27144adafcc
Windows installers	Python 2.7	Miniconda2 Linux 64-bit	48.7 MIB	b820dde1a0ba868c4c948fe6ace7300a252b33b5befd078a15d4a017476b8976
MacOSX installers		Miniconda2 Linux 32-bit	39.0 MiB	2e20ac4379ca5262e7612f84ad26b1a2f2782d0994facdecb28e0baf5174997
Linux installers				

Fig. 64: Miniconda installers for Linux

3. Click on the download link corresponding to:

Python 3.8 – Miniconda3 Linux 64-bit

Save the file. It will be saved as:

Miniconda3-latest-Linux-x86_64.sh

Note: You can verify the file's SHA256 checksum to ensure

²¹ https://docs.conda.io/en/latest/miniconda.html

it has been downloaded correctly. *How?*

2. Running the installer

Run the installer using the bash command:

```
bash Miniconda3-latest-Linux-x86_64.sh
```

This will print a welcome message:

```
Welcome to Miniconda3 py38_4.8.3
```

In order to continue the installation process, please review the license agreement. Please, press ENTER to continue

3. Reviewing licence agreement

Press the ENTER key to view the licence agreement. Scroll down to read the licence. Towards the end, you will notice a prompt:

```
Do you accept the license terms? [yes|no]
[no] >>> yes
```

You will need to type *yes* to accept the agreement and then press the ENTER key to proceed.

4. Confirming Miniconda install location

Next, you will be asked to provide a path to install Miniconda.

```
Miniconda3 will now be installed into this location:
/home/user/miniconda3
  - Press ENTER to confirm the location
  - Press CTRL-C to abort the installation
  - Or specify a different location below
[/home/user/miniconda3] >>>
```

Press ENTER here to accept the default value.

Installation will now proceed. When complete, you will notice a prompt asking if you would like to *initialize Miniconda* 3.

```
Do you wish the installer to initialize Miniconda3
by running conda init? [yes|no]
[no] >>> yes
```

Type yes and then press the ENTER key. This will add the conda command to your \$PATH.

As a result of this configuration, Conda base environment will be activated automatically when you open a terminal session. This can be disabled in the next step. *Why?*

5. Disabling auto-activation of base environment

Open a new terminal. Your shell prompt should now appear like the following:

```
(base) user@cookbook:~$
```

The (base) label at the beginning of the prompt, indicates that Conda base environment is now active.

To disable this behaviour, so you can activate the environment manually when you need it, run the following command:

conda config --set auto_activate_base false

6. Setting up channels

Channels provide additional software for Conda.

Conda's configuration includes a defaults²² channel. The *bioconda* and conda-forge²³ channels can also be added to access an even larger collection of software. The bioconda channel, for example, provides over 7000 packages of Bioinformatics software.

To add these channels to your configuration, you can run the commands below.

²² https://repo.anaconda.com/pkgs

²³ https://conda-forge.org/

Attention: You will need to run these commands in the same order as given below.

```
conda config --add channels defaults
conda config --add channels bioconda
conda config --add channels conda-forge
```

Installation and configuration of Conda is now complete.

You can now start using Conda to create environments and install packages from repositories.

3.5.3 Using Conda

In this short guide on using Conda, I will show you how to:

- 1. Create an environment
- 2. Activate the environment
- 3. Search, install and use packages using the NCBI BLAST+ program as an example
- 4. Remove an environment when you no longer need it

Note: A cheat sheet²⁴ with commonly used commands for working with Conda is available from the project's website.

Creating an environment

To create an environment, use the conda create command with the -n option, followed by a name for the environment — blast in this example:

conda create -n blast

²⁴ https://docs.conda.io/projects/conda/en/latest/user-guide/cheatsheet. html

Activating an environment

You can get a *list* of all environments using the command:

conda envs list

To activate an environment, use the conda activate command with the *name* of the environment:

conda activate blast

Searching, installing and using Packages

To search and install packages:

1. First, activate the environment, if you haven't done so already.

To demonstrate, I will activate the blast environment created earlier:

```
conda activate blast
```

2. To search for packages, open Anaconda.org²⁵ in a browser.

Type your search term in the Search Packages field and press the ENTER key (Fig. 65).

```
<sup>25</sup> https://anaconda.org/
```

O Search :: Ani		Search :: Anaconda.org — Mozilla Firefox + https://anaconda.org/search?q=blast	··· ☆	- ~ &
	ONDA. ORG			
blast				Q
▼ Filters Type: All >	- Downloads	Access: All ∽ ◆ Package (owner / package)	Platform: All ~	Platforms
9	446430	 bioconda / blast 2101 BLAST+ is a new suite of BLAST tools that util C++ Toolkit. 	izes the NCBI	linux-64 osx-64
0	35773	O bioconda / samblaster 0.126 Mark duplicates in and extract discordant and SAM files.	l split reads from conda	linux-64 osx-64
0	32262	O conda-forge / clblast 14.1 CLBlast is a modern, lightweight, performant OpenCL BLAS library written in C++11	and tunable conda	linux-64 osx-64 win-32 win-64

Fig. 65: Searching for a package on Anaconda.org

Alternatively, you can use the conda search command:

conda search blast

This will output matching packages:

```
Loading channels: done

# Name Version Build Channel

blast 2.2.31 1 bioconda

...

blast 2.9.0 pl526he19e7b1_7 bioconda

(continues on next page)
```

(continued from previous page)

blast 2.10.1 pl526he19e7b1_2 bioconda

3. To install the package, use the conda install command with the *name* and *version* number of the package.

Attention: You will need to use the *highest* version number of the program, obtained from search results. Otherwise, an older version might get installed.

conda install blast==2.10.1

4. Once installed, you can start using programs included with the package, for example:

(blast) user@cookbook:~\$ blastn -version

Output:

```
blastn: 2.10.1+
Package: blast 2.10.1, build Oct 14 2020 11:36:30
```

Deactivating an environment

When your work is complete, you can deactivate an environment. To do so, use the command:

conda deactivate

Your shell prompt will change to its default state i.e., without the name of the Conda environment — (blast) in this case.

Removing an environment

To remove an environment, when you no longer need it, use the command:

```
conda remove -n blast --all
```

Here -n is used to indicate the name of environment you would like to remove and --all removes all packages installed in that environment.

3.5.4 Notes

How to verify the installer's SHA256 checksum

 Navigate to the folder containing the installer file – Miniconda3-latest-Linux-x86_64.sh:

cd Downloads

2. Use the sha256sum command to verify the SHA256 checksum of the file:

sha256sum Miniconda3-latest-Linux-x86_64.sh

Output:

879457af6a0bf5b34b48c12de31d4df0ee2f06a8e68768e5758c3 →293b2daf688 Miniconda3-latest-Linux-x86_64.sh

The output of the sha256sum command should match the value listed on the downloads page.

Why disable auto-activation of base environment?

If you are installing packages using other methods, for example *Installing a Python package* from PyPI, there is a possibility that you might *accidentally* install the package in Conda base environment instead of the intended location.

Even if you disable auto-activation of the base environment, you

can activate it using the conda activate base command, when you need it.

3.6 Debian packages

If your software of interest is available as a *Debian package*, you can use the *gdebi* program to install it. If the software has any *dependencies*, they will be installed automatically.

Examples of software that can be installed using this method:

RStudio Desktop – an IDE for the R programming language

Modeller — a program for comparative modelling of protein three-dimensional structures

MEGA — Molecular Evolutionary Genetics Analysis

3.6.1 Requirements

Attention: This procedure installs software in system paths and so requires administrator privileges.

3.6.2 Installing a Debian package

To demonstrate the steps involved in installing a Debian package, I will download and install *RStudio Desktop* — an IDE for R, distributed as a Debian package.

1. Downloading Debian package

Open the RStudio project's download²⁶ page in a web browser.

Under Choose Your Version, click on the download button below RStudio Desktop (Open Source License) (Fig. 66).

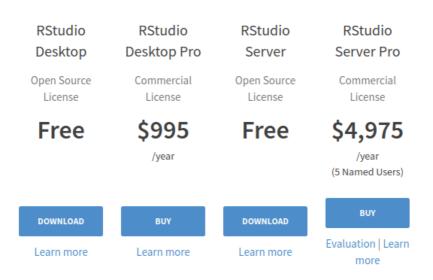


Fig. 66: Download RStudio Desktop (Open Source License)

This will take you to the installers section with information on

²⁶ https://rstudio.com/products/rstudio/download/

the current version (Fig. 67).





Fig. 67: RStudio Desktop installers

Note: Although the instructions in Fig. 67 state that you will need to install R before installing RStudio, you can safely *skip that step*.

The Gdebi program used here, will automatically install R, while installing RStudio.

Scroll down to the All Installers section.

Click on the download link corresponding to Ubuntu 18/Debian 10 (Fig. 68).

All Installers

Linux users may need to import RStudio's public code-signing key prior to installation, depending on the operating system's security policy.

RStudio requires a 64-bit operating system. If you are on a 32 bit system, you can use an older version of RStudio.

OS	Download	Size	SHA-256
Windows 10/8/7	🛓 RStudio-1.4.1103.exe	156.96 MB	c3384189
macOS 10.13+	🛓 RStudio-1.4.1103.dmg	152.77 MB	20148bd6
Ubuntu 16	🛓 rstudio-1.4.1103-amd64.deb	119.26 MB	f0857e27
Ubuntu 18/Debian 10	🛓 rstudio-1.4.1103-amd64.deb	120.30 MB	76864349
Fedora 19/Red Hat 7	🛓 rstudio-1.4.1103-x86_64.rpm	138.02 MB	8fcb2d29

Fig. 68: RStudio installers for different operating systems

In the dialog window that appears, select Save File and then click on the OK button (Fig. 69).

Linux for Biologists

	Downloa	d the RStudio IDE - R	Studio — Moz	illa Firefox		- a 😣
B Download the RS	Studio × +					
← → ⊂ ŵ	🔽 🔒 https:	//rstudio.com/produ	cts/rstu 🗉	··· ☆	⊻ III\ ⊡	tî ≡
All Insta		Opening rstudio-1.4.1	103-amd64.de	eb	8	
Linux users m depending or		n to open: .1103-amd64.deb ebian package (115 M	B)		ation,	
RStudio requi older version		//download1.rstudio.o			use an	
	Open with	GDebi Package Ins	taller (default)	~		
OS Windows 10/8/	Do this <u>a</u> ut	omatically for files like	e this from nov	v on.	- ^J IA-256	
macOS 10.13+			Cancel	ОК)148bd6	
Ubuntu 16	£	rstudio-1.4.1103-amd64.	deb	119.26 MB	f0857e27	
Ubuntu 18/Deb	ian 10 🕹	rstudio-1.4.1103-amd64.	deb	120.30 MB	76864349	
Fedora 19/Red	Hat 7 🛃	rstudio-1.4.1103-x86_64.	rpm	138.02 MB	8fcb2d29	

Fig. 69: Save installer file

Once the file download is complete, you can find it in your Downloads directory.

2. Installing downloaded package

Open file manager and navigate to your Downloads directory.

Double-click on the downloaded file (Fig. 70).

	Downloads - 🕫 📀
File Edit View	Go Bookmarks Help
$\leftrightarrow \rightarrow \uparrow$	/home/user/Downloads 🛛 .J Q 📰 🎞 🖽
 My Computer Home Desktop Documents Music Pictures Videos Videos Downloads Recent File System Trash Devices sf_Public Network Network 	amd64.deb
E E 3	"rstudio-1.4.1103-amd64.deb" selected (120.3 MB), Free space: 9.6 GB

Fig. 70: Downloaded Debian package

This will open the Gdebi application. Click on the Install Package button (Fig. 71).

	rstudio 1.4.1103			- 0	8
Requires the	e installation of 10 packages			Detai	ls
Maintainer Size:	: RStudio <info@rstudio.com> 805683 KiB</info@rstudio.com>		Instal	l Packag	ge
RStudio					2
productive supports di	a set of integrated tools designed with R. It includes a console, syr irect code execution, as well as t management.	ntax-highlight	ing edito	or that	

Fig. 71: Gdebi: Click on the Install Package button

You will be prompted to enter *your password*. Type in your password and click on the Authenticate button to proceed (Fig. 72).

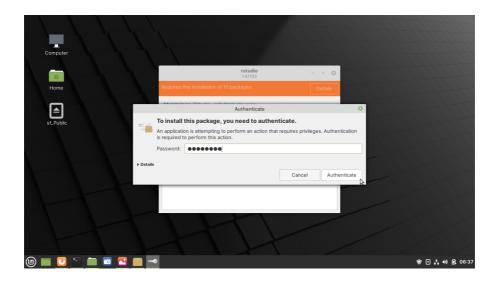


Fig. 72: Enter your password when prompted

As this package has additional dependencies, another dialog will appear listing these packages, which need to be installed in order for it to work.

Click on the Continue button to proceed (Fig. 73).

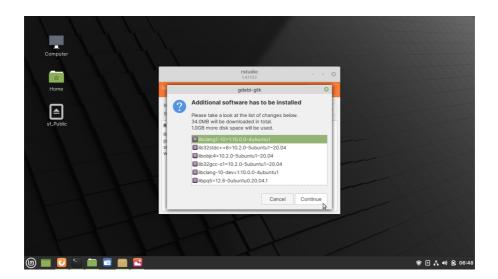


Fig. 73: Additional dependencies to be installed

Installation will now proceed (Fig. 74).

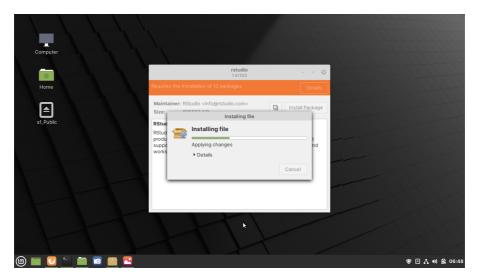


Fig. 74: Installation progress

When installation is complete, you will see a message Same version is already installed, at the top of the window (Fig. 75).

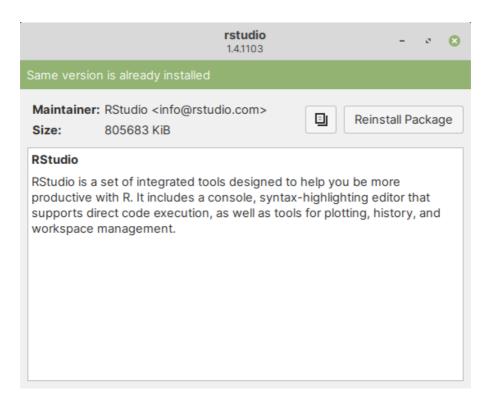


Fig. 75: Package installed successfully

3. Launching installed programs

You can launch installed programs from the Applications Menu (Fig. 76).

Note: This only applies to applications with a graphical user interface.



Fig. 76: Launching installed program from applications menu

The main window of the program will be displayed (Fig. 77).

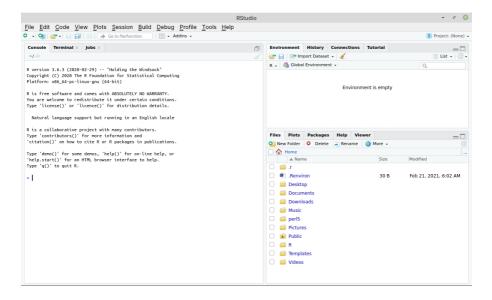


Fig. 77: Main window of RStudio Desktop

3.6.3 Upgrading installed software

Upgrading software installed from a Debian package, is similar to installation. When a new version of the program is available, download the package file (.deb) and then follow the steps in *Installing a Debian package*.

3.6.4 Removing installed software

You can follow the steps in *Removing installed software*, to search and remove packages installed in this manner.

3.6.5 Notes

The command-line version

You can use the *apt* package manager to install Debian packages on the command-line.

These programs need to be updated manually

Programs installed in this manner will not *usually* be updated automatically. So, this method should only be used for software not available using *The quick and easy method*.

If dependencies cannot be located, installation will fail

Installation of some programs might fail, if dependencies cannot be located in software repositories. In that case, you will need to find and install those packages manually and then attempt to install the program again.

Using the Linux command line

In this section, you will find an overview of the Linux command line, the shell and terminal programs, some commonly used commands, and a sample exercise.

4

4.1 Shell and Terminal

A *shell* is a program that provides an interface to the operating system's services. The most commonly used shell in Linux distributions is *Bash*.

A *terminal* program runs the shell and provides an interface for users to type commands.

The default terminal application in Linux Mint is Terminal (Fig. 78). You can launch it from the Applications Menu or by clicking on its icon in the Panel.

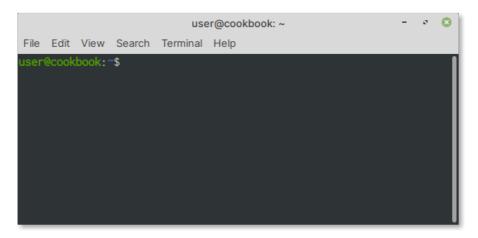


Fig. 78: A Terminal window

Once a terminal window is open, you can start typing commands at the \$ prompt.

For example, the following command:

pwd

Will output the current working directory:

/home/user

4.1.1 The shell prompt

The prompt user@cookbook:~\$ in Fig. 78, indicates the following:

user — username of the account

cookbook – the computer's hostname

- \sim short form for the user's home directory i.e., /home/user
- \$ a regular user account. For the root user, this will change to
 #

4.2 Commands — an overview

This section provides an overview of some commands that are used frequently on Linux systems.

Familiarity with these will help you navigate the file system and work with files, and directories.

4.2.1 Command options

A command might support additional options.

For example, the command:

ls

- prints a list of files in a directory, whereas:

ls -a

- will also print hidden files in that directory.

4.2.2 Getting help on using commands

In most cases, you can see the complete list of options a command supports using --help:

ls --help

Output:

```
Usage: ls [OPTION]... [FILE]...

List information about the FILEs (the current directory

→by default).

Sort entries alphabetically if none of -cftuvSUX nor --

→sort is specified.

Mandatory arguments to long options are mandatory for

→short options too.

-a, --all do not ignore entries

→starting with .

...
```

Note: To keep this discussion short, the examples in this section, only includes *some* options supported by a command.

4.2.3 date - display current date and time

date

Output:

Wed 10 Mar 2021 10:33:11 GMT

4.2.4 cd – change directory

To change into a directory, use cd followed by the name of that directory.

For example, to change into /home/user/Downloads, use:

cd Downloads

Note: When you log in or open a new terminal window, you will be placed in your home directory — /home/user, where user is your username.

You can verify your current directory using the pwd command discussed *earlier*:

pwd

/home/user/Downloads

cd with no arguments

No matter where you are in the file system, typing cd *without any arguments* will take you to your home directory.

```
user@cookbook:/usr/share/dict$ cd
user@cookbook:~$
```

Go to parent directory

Use cd .. to go to the parent directory.

For example, when you are in /home/user/Downloads and type:

cd ..

You will be taken to /home/user.

A single dot (.) refers to the *current* directory.

4.2.5 mkdir — create new directory

Use mkdir followed by the name of the directory you would like to create:

mkdir Workspace

Attention: The directory you're creating must not already exist or this command will not work.

As discussed *earlier*, directory names are case-sensitive, so a directory named Workspace is different from another named workspace.

Spaces in directory names

If there are spaces in the directory name, use double quotes, for example:

mkdir "Project Work"

Without that, two separate directories — Project and Work will be created.

4.2.6 rmdir — remove empty directory

Use rmdir followed by the name of the directory you would like to remove:

rmdir Workspace

Attention: This directory must be empty before it can be removed.

There should be no other files or directories within that directory.

4.2.7 ls — list files

To list files in a directory, use the ls command:

ls

Output:

```
Desktop Documents Downloads Music Pictures Public ☑

→Templates Videos
```

Listing hidden files

You can provide additional options to ls. It will change how the command works.

For example, to display hidden files and directories too, use:

ls -a

Output:

	.cache	Downloads	.local	Public
	.cinnamon	.gnupg	.bash_his	tory .
⊶config				
.bash_logout	Desktop	Pictures	.var	Videos
.bashrc	Documents	.linuxmint	.profile	

Getting a detailed file listing

To get a detailed listing of files, use:

ls -l

Output:

total 32								
drwxr-xr-x	2	user	user	4096	Feb	17	11:13	Desktop
drwxr-xr-x	2	user	user	4096	Mar	4	11:41	Documents
drwxr-xr-x	2	user	user	4096	Feb	17	11:13	Downloads
drwxr-xr-x	2	user	user	4096	Feb	17	11:13	Music
drwxr-xr-x	2	user	user	4096	Mar	4	11:27	Pictures
drwxr-xr-x	2	user	user	4096	Feb	17	11:13	Public
drwxr-xr-x	2	user	user	4096	Feb	17	11:13	Templates
drwxr-xr-x	2	user	user	4096	Feb	17	11:13	Videos

Combining multiple options

You can combine multiple options like this:

ls -la

Output:

total 144 drwxr-xr-x 19 user user 4096 Mar 12 10:00 . drwxr-xr-x 3 root root 4096 Feb 17 10:51 ..

(continues on next page)

(continued from previous page)

 -rw----- 1 user user
 190 Mar
 4 10:32 .bash_history

 -rw-r--r- 1 user user
 220 Feb
 17 10:51 .bash_logout

 -rw-r--r- 1 user user
 3771 Feb
 17 10:51 .bashrc

 drwx----- 17 user user
 4096 Mar
 3 19:28 .cache

 drwxrwxr-x
 4 user user
 4096 Feb
 17 11:40 .cinnamon

To see the list of all options that ls supports, use:

ls --help

4.2.8 cp – copy files

With the cp command, you can copy files or directories from one place (*source*) to another (*destination*).

Copying one file

To copy one file, use the following format:

```
cp source_file destination
```

Where source_file is the file you would like to copy and destination can *either* be a file name or a directory.

If destination is a file name

The copied file will have that file name.

For example:

```
cp /usr/share/dict/words /home/user/Documents/dictionary.
→txt
```

This will copy the words file from /usr/share/dict/ to /home/ user/Documents/ and save it as dictionary.txt.

If destination is a directory

The file will be copied *into* that directory with the *same* file name.

For example:

cp /usr/share/dict/words /home/user/Documents

This will copy the words file from /usr/share/dict/ to /home/ user/Documents/ with the same file name.

Copying multiple files

To copy multiple files, use the following format:

cp source_file1 source_file2 destination

Where source_file1 and source_file2 are the files you would like to copy. You can have *any* number of source files. Here, *destination* is the directory where you would like to copy source files into.

For example:

```
cp /usr/share/dict/words /usr/share/dict/spanish /home/
→user/Documents
```

This will copy the words and spanish dictionary files from /usr/ share/dict/into /home/user/Documents.

Copying directories

You can copy entire directories using the -r (recursive) option.

For example:

cp -r /usr/share/dict /home/user/Documents

This will copy the /usr/share/dict directory and its contents to the Documents directory.

4.2.9 cat - display contents of files or combine them

With the cat command, you can view the contents of a file on the screen or combine contents of multiple files.

View contents of a file

To view the contents of a file, use cat, followed by the name of the file:

```
cat /usr/share/dict/words
```

A A's AMD AMD's AOL AOL's AWS AWS's Aachen

This will display the *entire contents* of the file.

Combine contents of files

If you include multiple file names in cat, it will combine them and print their contents on the screen.

If you would like to save the output to a file instead, use the following format:

cat file1.txt file2.txt > files.txt

The > operator redirects *standard output* to the file name following it.

4.2.10 less — view and navigate file contents

With the less command, you have more control when viewing a file. It allows you to scroll up and down the file and provides features like searching the file using keywords.

To view the contents of a file, use less, followed by the name of the file:

```
less /usr/share/dict/words
```

When the file is open, it will appear as in Fig. 79.

user@cookbook: ~						-	ø	8	
File	Edit	View	Search	Terminal	Help				
A AMD AMD's AOL AOL's AWS AWS's Aache Aache	s s en								

Fig. 79: The words file open in less command

At the : prompt, you can type commands that less will understand.

Navigating the file

You can scroll down the file by pressing the ENTER key.

Alternatively, you can use the PgUp and PgDn keys to scroll one page at a time.

Searching the file

You can search a file while viewing it in less.

To do this:

- 1. Type / (forward slash) key
- 2. Type the text you would like to search
- 3. Press the ENTER key
- 4. If there are matching results, they will be highlighted

Quitting the less command

To quit the less command, type q at the prompt.

4.2.11 head — print first few lines of a file

With the head command, you can view the first few (default: 10) lines of a file.

For example:

head /usr/share/dict/words

Will produce the following output:

A A's AMD AMD's AOL AOL's AWS AWS's Aachen Aachen's

4.2.12 tail - print last few lines of a file

With the tail command, you can view the last few (default: 10) lines of a file.

For example:

tail /usr/share/dict/words

élan's émigré émigrés épée épée's épées étude étude's études

The tail and the head command discussed *earlier*, are useful when you want to quickly view the contents of a *large* text file.

In both cases, you can control the *number of lines* displayed, using the -n option, instead of the default value (10).

For example:

tail -n 5 /usr/share/dict/words

will display the last 5 lines of the file.

4.2.13 mv — move a file or directory

With the mv command, you can move a file or directory from one location (source) to another (destination). You can choose to keep the existing file or directory name or rename them.

The basic format of the command is:

```
mv source destination
```

A safer approach is to add the -iv options to the command:

```
mv -iv source destination
```

With -i (*interactive*), mv will require your confirmation before overwriting a file or directory, if it exists already in destination.

-v (verbose) will print the command's actions on the screen.

For convenience, you can *add an alias*.

Sample files

To follow the examples below, you will need to copy the following files into your home directory using the *cp* command:

```
cp -v /usr/share/dict/words ~
cp -rv /usr/share/doc/bash ~
```

~ is a shortcut for home directory.

Moving a file or directory

The simplest use case is to move a file or directory from one location (directory) to another.

Moving a File

For example, to move the words file copied *above* into your Documents directory, use:

mv -iv words Documents/

Output:

renamed 'words' -> 'Documents/words'

Moving a directory

Similarly, to move the bash directory copied *above* into your Documents directory, use:

mv -iv bash Documents/

Output:

```
renamed 'bash' -> 'Documents/bash'
```

In both cases, the file or directory name will not be changed.

Renaming a file or directory

In this case, you would like to rename a file or directory.

Renaming a file

To rename the words file copied *above* to dictionary.txt, use:

mv -iv words dictionary.txt

Alternatively, to move it into your Documents directory and rename it at the same time, use:

mv -iv words Documents/dictionary.txt

Renaming a directory

To rename the bash directory copied *above* into bash-commands, use:

mv -iv bash bash-commands

Notes

What happens if a file exists?

You will notice a prompt requesting you for confirmation to overwrite the file. Type y and press the ENTER key to proceed:

```
mv: overwrite 'Documents/words'? y
renamed 'words' -> 'Documents/words'
```

To cancel, simply press ENTER key at the prompt.

What happens if a directory exists?

mv will overwrite a directory only if it is empty. You can either:

- *copy* files into destination directory or
- rename the destination directory

Adding an alias for mv

Rather than typing mv -iv, every time you need to use the command, you can add an *alias* for the command in your ~/. bash_aliases file.

For example:

```
alias mv='mv -iv'
```

Now, when you type mv, you will actually be running mv -iv.

4.2.14 rm — remove files or directories

With the rm command, you can remove (or delete) files or directories.

The basic format of the command is:

rm source

A safer approach is to add the -iv options to the command:

```
rm -iv source
```

With -i (*interactive*), rm will require your confirmation before deleting a file or directory.

-v (verbose) will print the command's actions on the screen.

For convenience, you can *add an alias*.

Sample files

To follow the examples below, you will need to:

 Copy the following files into your home directory using the *cp* command:

```
cp -v /usr/share/dict/words ~
cp -rv /usr/share/doc/bash ~
```

~ is a shortcut for home directory.

2. Create an empty directory:

mkdir empty-dir

Removing files

To remove a file, for example, the words file copied *above*, you can use:

rm -iv words

Output:

```
rm: remove regular file 'words'? y
removed 'words'
```

Removing directories

Removing empty directories

If the directory is empty, you can remove it using the -d option:

```
rm -d empty-dir
```

Alternatively, you can use the *rmdir* command:

rmdir empty-dir

Removing directories with content

If the directory has some content i.e., files or subdirectories, you will need to add the -r (recursive) option.

For example, using the bash directory copied *above*:

rm -ivr bash

This command will ask for your confirmation for deleting every file in the directory and then delete it:

```
rm: descend into directory 'bash'? y
rm: remove regular file 'bash/RBASH'? y
removed 'bash/RBASH'
....
rm: remove regular file 'bash/README.gz'? y
removed 'bash/README.gz'
rm: remove directory 'bash'? y
removed directory 'bash'
```

Instead of -i, you could use the -I option, which will only prompt once, when removing directories recursively:

rm -Ivr bash

Output:

```
rm: remove 1 argument recursively? y
removed 'bash/RBASH'
```

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removed 'bash/README.gz'
removed directory 'bash'

If you are *completely sure* you do not need the directory and its contents, you can *force* its removal using the -f option:

rm -vrf bash

rm will delete the directory without confirmation.

Notes

Adding an alias for rm

Rather than typing rm -iv, every time you need to use the command, you can add an *alias* for the command in your ~/. bash_aliases file.

For example:

```
alias rm='rm -iv'
```

Now, when you type rm, you will actually be running rm -iv.

4.2.15 echo — display text or values of variables

With the echo command, you can print text or the values of *environment variables* on the screen.

The basic format of the command is:

```
echo text_or_variable
```

Printing text

To print text on the screen, use echo followed by the text you would like to display.

echo "Hello, This is echo!"

Output:

Hello, This is echo!

Printing values of environment variables

You can also use echo to display values of your environment variables.

For example:

echo \$PATH

The \$ in PATH indicates, it is a variable.

Output:

```
/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/

→bin:/usr/games:/usr/local/games:/snap/bin
```

PATH contains the list of paths (directories) that will be searched for locating programs or commands.

You can set or modify environment variables in your ~/.bashrc.

4.3 Other useful commands

These are some additional commands that you might find useful.

4.3.1 df – report disk usage

The df command will report used and available disk space on all storage devices connected to the system.

For example, to find the amount of disk space used in /- the root filesystem, you can use the command:

df -h /

Output:

Filesystem	Size	Used	Avail	Use%	Mounted	on
/dev/mapper/vgmint-root	28G	6.9G	20G	26%	/	

The -h option makes the output human-readable. Without this, available disk space will be reported as 20600196 instead of 20G.

4.3.2 du — estimate disk usage of files or directories

Calculate the amount of disk space used by files or directories.

For example, to calculate the amount of disk space used by files in your home directory, use the command:

du -sh ~

Output:

7.4G .

The -s option prints a summary instead of printing space used by individual files.

-h makes the output human-readable.

4.3.3 find — search for files

Search for files using their file name, file type etc.,

For example, to find files in the home directory with .bash in their name, use the command:

find ~ -name ".bash*"

Output:

/home/user/.bashrc
/home/user/.bash_history
/home/user/.bash_logout

Note: The ~ here is a shortcut for home directory.

The asterisk symbol (*) in .bash* acts as a wildcard.

The find command does not use a database, so the search will be slower when compared to locate. However, it can identify files that were created or modified recently.

4.3.4 free — view free and used memory

With free, you can find the amount of free and used memory (RAM (Random Access Memory)) and swap space.

Usage:

free -h

Output:

total	used	free	shared 🛛
available			
3.8Gi	618Mi	1.3Gi	7.0Mi 🛛
3.0Gi			
979Mi	ØB	979Mi	
	available 3.8Gi 3.0Gi	available 3.8Gi 618Mi 3.0Gi	available 3.8Gi 618Mi 1.3Gi 3.0Gi

The -h option makes the output human-readable with corresponding units displayed. In the example above, the amount of free physical memory (RAM) is 1.3 GiB (Gibibytes).

4.3.5 locate — find files using their names

Search for files using their file names. This method is quick as it uses a file name database.

For example:

locate bashrc

Output:

/etc/bash.bashrc
/etc/skel/.bashrc
/home/user/.bashrc
...

Note: This method might not find files that were created or modified recently.

Newer files might not yet be included in the database. To update the database manually, you can run the command:

sudo updatedb

Alternatively, you can use the *find* command to search for new files.

4.3.6 which — locate a command

The which command prints the complete path to a command, if it exists in the search path i.e., \$PATH.

For example:

which python3

Output:

/usr/bin/python3

4.4 Editing text files using nano

GNU nano is a command-line text editor with features like undo/redo, syntax colouring, interactive search and replace and more.

To open the program, type nano in a terminal session.

4.4.1 Create new file

To create a new file, use nano followed by the name of the file you would like to create.

For example:

```
nano exercise.txt
```

This will open the file for writing (Fig. 80).



Fig. 80: Creating a file in nano

You can start typing text at this stage.

4.4.2 Pasting text from clipboard

To copy and paste text from a different program, for example, a web browser into a file you are editing in nano, do the following:

- Copy the text from the program to clipboard using Ctrl + c
- 2. In nano, move the cursor to the position where you would like to paste the text
- 3. Use the Shift + Ctrl + v keyboard shortcut to paste the text

4.4.3 Saving changes

To save the file, use the shortcut Ctrl + o.

This corresponds to the ^O Write Out function displayed at the bottom (Fig. 81). The ^ here refers to the Ctrl key.

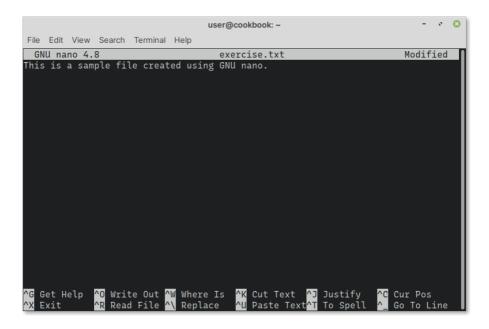


Fig. 81: To save changes use the Write Out function

A prompt like the following will be displayed at the bottom (Fig. 82):

File Name to Write: exercise.txt

	user@cookbook: ~	- v 🔇
File Edit View Search Terminal Help		
GNU nano 4.8	exercise.txt	Modified
This is a sample file created usin	g GNU nano.	
File Name to Write: exercise.txt		
<mark>^G</mark> Get Help M-D DOS Format		<mark>M-B</mark> Backup File
<mark>^C</mark> Cancel M-M Mac Format	M-P Prepend	<mark>^T</mark> To Files

Fig. 82: Enter a file name to save the file

Press the ENTER key to accept the default value — the original file name.

4.4.4 Exit nano

To exit nano, use the Ctrl + x shortcut.

If there are no changes, nano will close. If there are unsaved changes, it will prompt you to save them (Fig. 83).

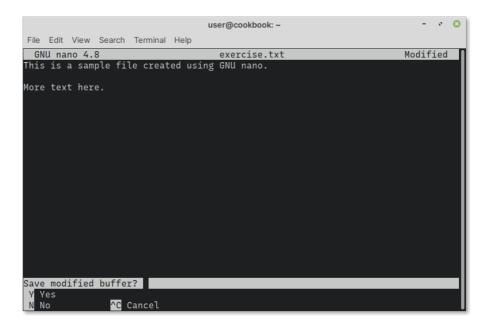


Fig. 83: Confirmation to save changes to file

Type y to save changes or n to discard them.

4.5 Exercise — using the command-line

This is an exercise in using the command-line to accomplish a task. You will be making use of the commands *discussed earlier*.

Task

Given a protein sequence, identify matching sequences from a protein sequence database.

Approach

Using programs in the NCBI BLAST+ package, you can search a database of sequences using sequence (query) to identify matching sequences.

4.5.1 Summary of steps

- 1. Install NCBI BLAST+
- 2. Download protein query sequence
- 3. Download protein sequence database and format it
- 4. Search database using the query sequence

4.5.2 Get sample data

To proceed, you will need to download the protein query sequence and database used in this exercise.

Download query sequence

The protein query sequence used in this exercise is *Spike gly-coprotein* from Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). It is available from UniProtKB²⁷ — the protein knowledge base.

The database identifier for this protein is P0DTC2²⁸. You can download the sequence in FASTA format from the entry page or using this direct link:

https://www.uniprot.org/uniprot/P0DTC2.fasta

Download protein database

The database used in this exercise is UniProtKB Swiss-Prot²⁹. It is a manually annotated database of protein sequences with added functional information.

You can download the entire database as a compressed FASTA format file from the downloads³⁰ page on the website.

²⁷ https://uniprot.org/uniprot/

²⁸ https://www.uniprot.org/uniprot/P0DTC2

²⁹ https://uniprot.org/uniprot/?query=reviewed:yes

³⁰ https://www.uniprot.org/downloads

4.5.3 Install NCBI BLAST+ package

Attention: This procedure installs software in system paths and so requires administrator privileges.

NCBI BLAST+ is available in the Linux package repositories. You can install it using apt:

sudo apt install ncbi-blast+

Type y when prompted to continue.

```
[sudo] password for user:
Reading package lists... Done
Building dependency tree
Reading state information... Done
The following additional packages will be installed:
    libmbedcrypto3 libmbedtls12 libmbedx509-0 ncbi-data
The following NEW packages will be installed:
    libmbedcrypto3 libmbedtls12 libmbedx509-0 ncbi-blast+☑
    hncbi-data
0 upgraded, 5 newly installed, 0 to remove and 0 not☑
    jupgraded.
Need to get 14.9 MB of archives.
After this operation, 75.0 MB of additional disk space☑
    will be used.
Do you want to continue? [Y/n] y
```

4.5.4 Download query sequence

You can follow these steps to download the query sequence:

- 1. Create new directory
- 2. Change into it
- 3. Download query sequence
- 4. View the downloaded sequence (optional)

Create new directory – mkdir

To keep the input and output files related to this project together, create a new directory in your home directory using the *mkdir* command.

```
mkdir -p ~/projects/sars-cov-2
```

Here:

~ is shortcut for home directory.

-p creates parent directories if necessary. In this case, the projects directory does not exist, so it is also created.

Change directory — cd

Change into the newly created directory using the *cd* command:

```
cd ~/projects/sars-cov-2
```

Download sequence - wget

To download the sequence file, you can use the wget command with the link to download as the argument. In this case, the link to download is the URL corresponding to the FASTA format file (see *sample data*):

```
wget https://www.uniprot.org/uniprot/P0DTC2.fasta
```

When the download is complete, you can use the *ls* command to verify if the file exists:

ls -l

Output:

```
total 4
-rw-rw-r-- 1 user user 1414 Feb 10 00:00 PODTC2.fasta
```

View downloaded sequence - cat or less

Since PODTC2.fasta is in FASTA format — a plain-text format, you can use the *cat* command to view the file's contents:

cat P0DTC2.fasta

Output:

>sp|P0DTC2|SPIKE_SARS2 Spike glycoprotein OS=Severe acute →respiratory syndrome coronavirus 2 OX=2697049 GN=S PE=1 →SV=1

MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVYYPDKVFRSSVLHSTQDLFLPFFS NVTWFHAIHVSGTNGTKRFDNPVLPFNDGVYFASTEKSNIIRGWIFGTTLDSKTQSLLIV NNATNVVIKVCEFQFCNDPFLGVYYHKNNKSWMESEFRVYSSANNCTFEYVSQPFLMDLE GKQGNFKNLREFVFKNIDGYFKIYSKHTPINLVRDLPQGFSALEPLVDLPIGINITRFQT LLALHRSYLTPGDSSSGWTAGAAAYYVGYLQPRTFLLKYNENGTITDAVDCALDPLSETK CTLKSFTVEKGIYOTSNFRVOPTESIVRFPNITNLCPFGEVFNATRFASVYAWNRKRISN CVADYSVLYNSASFSTFKCYGVSPTKLNDLCFTNVYADSFVIRGDEVRQIAPGQTGKIAD YNYKLPDDFTGCVIAWNSNNLDSKVGGNYNYLYRLFRKSNLKPFERDISTEIYQAGSTPC NGVEGFNCYFPLQSYGFQPTNGVGYQPYRVVVLSFELLHAPATVCGPKKSTNLVKNKCVN FNFNGLTGTGVLTESNKKFLPF00FGRDIADTTDAVRDP0TLEILDITPCSFGGVSVITP GTNTSNQVAVLYQDVNCTEVPVAIHADQLTPTWRVYSTGSNVFQTRAGCLIGAEHVNNSY ECDIPIGAGICASYOTOTNSPRRARSVASOSIIAYTMSLGAENSVAYSNNSIAIPTNFTI SVTTEILPVSMTKTSVDCTMYICGDSTECSNLLLQYGSFCTQLNRALTGIAVEQDKNTQE VFAQVKQIYKTPPIKDFGGFNFSQILPDPSKPSKRSFIEDLLFNKVTLADAGFIKQYGDC LGDIAARDLICAQKFNGLTVLPPLLTDEMIAQYTSALLAGTITSGWTFGAGAALQIPFAM QMAYRFNGIGVTQNVLYENQKLIANQFNSAIGKIQDSLSSTASALGKLQDVVNQNAQALN TLVKQLSSNFGAISSVLNDILSRLDKVEAEVQIDRLITGRLQSLQTYVTQQLIRAAEIRA SANLAATKMSECVLGQSKRVDFCGKGYHLMSFPQSAPHGVVFLHVTYVPAQEKNFTTAPA ICHDGKAHFPREGVFVSNGTHWFVTQRNFYEPQIITTDNTFVSGNCDVVIGIVNNTVYDP LQPELDSFKEELDKYFKNHTSPDVDLGDISGINASVVNIQKEIDRLNEVAKNLNESLIDL QELGKYEQYIKWPWYIWLGFIAGLIAIVMVTIMLCCMTSCCSCLKGCCSCGSCCKFDEDD SEPVLKGVKLHYT

For more control, you can use the *less* command instead of cat.

4.5.5 Download protein sequence database

You can follow these steps to download and prepare the protein sequence database:

- 1. Create new directory
- 2. Change into it
- 3. Download the database archive
- 4. Uncompress (or extract) the database archive
- 5. Format the database

Create new directory — mkdir

In order to keep all BLAST databases in one location, create a directory to store them using the *mkdir* command:

mkdir ~/databases

Change directory — cd

Change into the newly created directory using the *cd* command:

```
cd ~/databases
```

Download the database archive — wget

Visit the database downloads³¹ page on the UniProt website.

Navigate to the UniProtKB section.

Right-click on the fasta download link corresponding to Reviewed (Swiss-Prot) and then copy it to clipboard (Fig. 84).

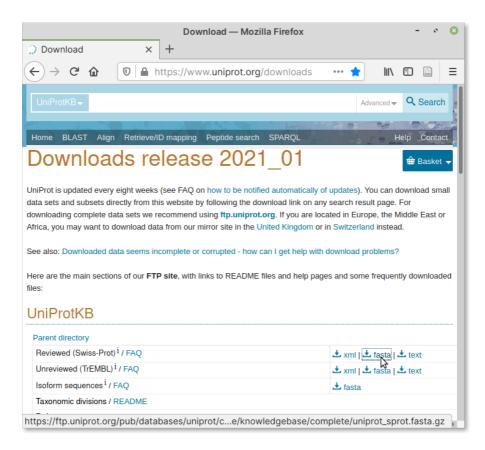


Fig. 84: Download link for Swiss-Prot database

To download the database, you can use the wget command with

³¹ https://www.uniprot.org/downloads

the link to download as the argument:

```
wget https://ftp.uniprot.org/pub/databases/uniprot/

→current_release/knowledgebase/complete/uniprot_sprot.

→fasta.gz
```

When the download is complete, you will find a file named uniprot_sprot.fasta.gz in the current directory. You can use the *ls* command to verify if it exists:

ls -lh

Output:

```
total 86M
-rw-rw-r-- 1 user user 86M Feb 10 15:00 uniprot_sprot.
⇔fasta.gz
```

Since this file is in a compressed format (.gz), you will need to uncompress it before proceeding.

Uncompress the database archive — gunzip

To uncompress (or extract) the database archive file downloaded in the previous step, you can use the gunzip command.

Note: By default, gunzip will remove the original compressed file after extraction.

If you would like to keep the original file (.gz), you can include

the -k (keep input files) option with gunzip.

Provide the file name of the downloaded file as the argument:

gunzip uniprot_sprot.fasta.gz

When the extraction is complete, you will find the database file in FASTA format in the same directory:

ls -lh

Output:

```
total 267M
-rw-rw-r-- 1 user user 267M Feb 10 15:00 uniprot_sprot.
→fasta
```

View the database

Since this extracted database file is large, you can use the *head* command to view the first few lines of the file:

```
head -n 5 uniprot_sprot.fasta
```

Output:

```
>sp|Q6GZX4|001R_FRG3G Putative transcription factor 001R

→0S=Frog virus 3 (isolate Goorha) 0X=654924 GN=FV3-001R

→PE=4 SV=1
```

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MAFSAEDVLKEYDRRRRMEALLLSLYYPNDRKLLDYKEWSPPRVQVECPKAPVEWNNPPS EKGLIVGHFSGIKYKGEKAQASEVDVNKMCCWVSKFKDAMRRYQGIQTCKIPGKVLSDLD AKIKAYNLTVEGVEGFVRYSRVTKQHVAAFLKELRHSKQYENVNLIHYILTDKRVDIQHL EKDLVKDFKALVESAHRMRQGHMINVKYILYQLLKKHGHGPDGPDILTVKTGSKGVLYDD

Alternatively, you can use the *less* command to view it one page at a time:

```
less uniprot_sprot.fasta
```

If you would like to count the number of sequences in the database, you can use the grep command.

grep ">" -c uniprot_sprot.fasta

Output:

564277

The -c option of grep, counts the number of times the given search string (> in this case) occurs in the input file.

Note: A sequence in a FASTA format should start with the > character. Hence, counting the number of times it occurs gives the number of sequences in the file.

You can now proceed towards formatting the database.

Format the database — makeblastdb

The database needs to be formatted before it can be used in a BLAST search. You can format it using the makeblastdb command, which is part of the NCBI BLAST+ package.

The command has multiple options. Here is an example:

```
makeblastdb -in uniprot_sprot.fasta -parse_seqids \
-title "Swiss-Prot" -dbtype prot -out swissprot
```

Note: The \ character splits the long command into multiple lines.

Output:

```
Building a new DB, current time: 03/24/2021 15:12:50

New DB name: /home/user/databases/swissprot

New DB title: Swiss-Prot

Sequence type: Protein

Keep MBits: T

Maximum file size: 100000000B

Adding sequences from FASTA; added 564277 sequences in 47.

→507 seconds.
```

What the options mean:

-in File name containing input sequences.

-parse_seqids Parse sequence identifiers from the input file. These will be displayed in search results. -title A descriptive name for this database.

- -dbtype The type of input sequences acceptable values are prot (for protein) and nucl (for nucleotide) sequences.
- -out The value here will be used to name the output files. This is also the name you will need to use for the database while doing a search (see *New DB Name*) in output.

When formatting is complete, you will notice the following files in the databases directory:

ls -lh

Output:

total 585M								
-rw-rw-r	1	user	user	100M	Mar	24	15:13	swissprot.phr
-rw-rw-r	1	user	user	4.4M	Mar	24	15:13	swissprot.pin
-rw-rw-r	1	user	user	2.2M	Mar	24	15:13	swissprot.pog
-rw-rw-r	1	user	user	18M	Mar	24	15:13	swissprot.psd
-rw-rw-r	1	user	user	411K	Mar	24	15:13	swissprot.psi
-rw-rw-r	1	user	user	195M	Mar	24	15:13	swissprot.psq
-rw-rw-r	1	user	user	267M	Feb	10	15:00	uniprot_sprot.
⊶fasta								

4.5.6 Search database using query sequence

With the query sequence downloaded and the database downloaded and formatted, you can start performing a BLAST search.

First, change into the directory containing the query sequence:

```
cd ~/projects/sars-cov-2
```

Now run the blastp command using the query sequence and the complete path to the database:

```
blastp -query P0DTC2.fasta \
-db /home/user/databases/swissprot \
-out blastp-results.txt \
-outfmt "7 sacc stitle qlen slen pident"
```

What the options mean:

-query Path to the query sequence.

- -db Complete path of the sequence database.
- -out File to save results to.
- -outfmt Format of the output file. This will use format option 7 (tab-delimited text) and include the following information:
 - accession number and description of matching sequences (sacc and stitle),
 - query and subject sequence lengths (qlen and slen)
 - percentage identity of the match (pident).

When the database search is complete, you can open blastp-results.txt to view the results:

```
less -S blastp-results.txt
```

The -S option of the less command disables word-wrap.

Output:

```
# BLASTP 2.9.0+
# Query: sp|P0DTC2|SPIKE_SARS2 Spike glycoprotein
→OS=Severe acute respiratory syndrome coronavirus 2
→0X=2697049 GN=S PE=1 SV=1
# Database: /home/user/databases/swissprot
# Fields: subject acc., subject title, query length,
→ subject length, % identity
# 88 hits found
PØDTC2
           Spike glycoprotein OS=Severe acute
→respiratory syndrome coronavirus 2 OX=2697049 GN=S PE=1
→SV=1 1273
              1273
                      100.000
           Spike glycoprotein OS=Severe acute
P59594
→respiratory syndrome coronavirus OX=694009 GN=S PE=1
→SV=1
         1273
                 1255
                         76.038
           Spike glycoprotein OS=Bat coronavirus HKU3
03LZX1
→0X=442736 GN=S PE=3 SV=1
                              1273
                                      1242
                                              76.041
           Spike glycoprotein OS=Bat coronavirus Rp3/
Q3I5J5
→2004 0X=349344 GN=S PE=1 SV=1 1273
                                       1241
                                               75.334
           Spike glycoprotein OS=Bat coronavirus 279/
Q0Q475
→2005 OX=389167 GN=S PE=3 SV=1 1273
                                       1241
                                               74.745
. . .
```

4.6 Notes

4.6.1 Adding directories to PATH

The PATH variable stores the list of directories that will be searched to locate commands you type. If you have a *command* that is stored in a directory that is not on this list, you will need to add it to PATH.

You can display the current value of PATH using the *echo* command:

echo \$PATH

Output:

```
/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/

→bin:/usr/games:/usr/local/games:/snap/bin
```

To modify PATH and add a directory, you can follow the steps below. This example adds /home/user/.local/bin to PATH.

Attention: You will need to be careful while editing PATH.

You will also need to ensure that it includes \$PATH in the list. Otherwise, you will not be able to access any commands!

- 1. Open \$HOME/.bashrc in a *text editor*.
- 2. Add the following lines at the end of the file. Add the directory you wish to add separated by a colon. The list should end in \$PATH.

```
PATH=/home/user/.local/bin:$PATH
export PATH
```

Note: If a line with PATH exists already in the file, update it instead.

3. Verify the change using echo:



Output:

```
/home/user/.local/bin:/usr/local/sbin:/usr/local/
→bin:/usr/sbin:/usr/bin:/sbin:/bin:/usr/games:/usr/
→local/games:/snap/bin
```

When you log in again or open a new terminal session, commands in /home/user/.local/bin will be accessible.

4.6.2 Dealing with spaces in file names

When you create a new file or directory, it is a good idea to *not use spaces* in the file or directory name. This is especially useful while working with these files or directories in the command-line. Instead, you can use an underscore (_) or hyphen (-) to separate words in file names.

If you do have to work with file or directory names containing spaces, you can use quotes around the file or directory name.

For example:

```
mkdir "Sample Data"
```

To change into the Sample Data directory, use:

```
cd "Sample Data"
```

Print current directory:

pwd

Output:

/home/user/Sample Data

This would have been simpler if the directory name is sample-data. You will not need to use quotes in that case.

Getting started with Galaxy

The Galaxy³² project enables researchers to perform computational analyses using a web interface.

You can use the service online at http://usegalaxy.org/ or any of the other available public servers³³.

The software powering the servers itself, is available under an open-source licence. You can download it and set up a local instance on your computer.

³² https://galaxyproject.org/

³³ https://galaxyproject.org/use/

5.1 Why use Galaxy?

These are *some* advantages of using Galaxy.

You can:

- **Upload your data** and perform analysis using a *web interface*.
- **Use included tools** or install additional ones from the Galaxy tool shed (needs a *local instance*).
- Use history functionality to keeps track of the jobs¹ you run. This gives you the possibility to run them again at a later time (reproducibility).
- **Create workflows** by combining multiple tools. The output of one tool can be used as input for another.
- **Share your data** with other users. This includes histories, workflows etc.,

¹ Commands run with additional arguments, if any, along with input and output file paths.

5.1.1 What can you use Galaxy for?

These are some tasks you can accomplish using Galaxy:

- Get data from various sources (databases)
- Manipulate text data
- Convert between file formats
- Statistics
- Sort and filter data

Note: The *exercise* in *Using the Linux command line* chapter, can be reproduced using Galaxy, without the need to use the command line or install software.

You only need your input data — query sequence and the protein sequence database.

5.1.2 Why run Galaxy on your computer?

Running Galaxy on your computer i.e., a *local instance*, has some advantages:

- **Data storage is local** on your computer, whereas, if you use a public instance, it will be stored on a server, possibly un-encrypted².
- Access more tools that are not installed on public servers by installing them on your local instance.
- **CPU and storage limits** are dependent on your computer, whereas on public servers, there are limits on CPU and storage usage per user².

² This is the case on https://usegalaxy.org — the main Galaxy instance. For more information, please read the https://galaxyproject.org/ main/#user-data-and-job-quotas.

5.2 Running Galaxy on your computer

To run a local instance of Galaxy on your computer, you will need to:

- 1. Check if your computer meets all requirements
- 2. Get the latest release of Galaxy
- 3. Create a Python virtual environment
- 4. Start Galaxy

At this stage, you will be able to open Galaxy's web interface in a browser and start using the tools included.

Note: To make use of all the features that Galaxy offers like installing additional tools, you will also need to do the following:

- 5. Register a user account
- 6. Grant administrator privileges for user

5.2.1 Check system requirements

Before running Galaxy, you will need to:

- 1. Install Git and Python virtualenv module
- 2. Check if there is enough free disk space
- 3. Ensure that a Conda environment is not active

Install Git and Python virtualenv module

Git is necessary for getting the latest version of Galaxy's source code from GitHub. Python virtualenv module is necessary to set up an isolated virtual environment for running Galaxy.

To install them, use *Software Manager* or *apt*, and search and install the following packages:

- 1. git
- 2. python3-venv

Check free disk space

You will need *at least* 5 GB of free disk space for the initial setup. More space will be needed for your analyses and for the tools you might install from the Galaxy tool shed.

To check available disk space, you can use the Disk Usage Analyzer application or the *df* command.

Ensure a Conda environment is not active

Note: If you are not using Conda, you can ignore this requirement and proceed to the next step:

-> Getting the latest release of Galaxy

If you are using Conda, please make sure an environment is not active before the *Starting Galaxy* step.

You can deactivate an active Conda environment using the command:

conda deactivate

Although it is possible to install Galaxy using an existing Conda installation, it is simpler to create and use a virtual environment using Python's venv module.

-

With all the requirements satisfied, you can proceed towards getting the latest release of Galaxy using Git.

5.2.2 Getting the latest release of Galaxy

Create a directory to set up Galaxy and change into it:

```
mkdir ~/programs
cd ~/programs
```

Here ~ is a shortcut for your home directory.

Note: This directory is not specific for Galaxy.

You can use it for installing or storing other programs too.

Get the latest release of Galaxy from the project's repository on GitHub. The latest release at the time of this writing is **21.01**.

You can get (or clone) the repository using the git clone command:

```
git clone -b release_21.01 https://github.com/

→galaxyproject/galaxy.git
```

The -b option of git clone, checks out the specified Git branch — release_21.01 in this case.

Output:

```
Cloning into 'galaxy'...
remote: Enumerating objects: 364, done.
remote: Counting objects: 100% (364/364), done.
```

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```
remote: Compressing objects: 100% (232/232), done.
remote: Total 497693 (delta 184), reused 237 (delta 131),
→pack-reused 497329
Receiving objects: 100% (497693/497693), 520.44 MiB | 3.
→89 MiB/s, done.
Resolving deltas: 100% (391502/391502), done.
Updating files: 100% (5826/5826), done.
```

This will take some time depending on your network connection. Once complete, you will find a directory named galaxy in the current directory.

Next, you will need to create a Python virtual environment.

5.2.3 Creating a Python virtual environment

In this step, you will use Python 3 venv module to create an isolated virtual environment for Galaxy.

Note: For a detailed guide on creating and using virtual environments, read:

-> Python virtual environments

To create the virtual environment:

1. Change into the galaxy directory:

cd galaxy

2. Create virtual environment using .venv as the name.

```
python3 -m venv .venv
```

Attention: The dot (.) in .venv, is important.

3. Activate the virtual environment:

```
source .venv/bin/activate
```

Your shell prompt will now change to include (.venv):

(.venv) user@cookbook:~/programs/galaxy\$

4. Install or upgrade Python build tools:

```
pip3 install -U pip setuptools wheel
```

This step is necessary, so additional packages will build and install without any issues.

5. Finally, exit the virtual environment:

deactivate

In the *next step*, the start-up script will detect this environment and use it to install all *dependencies* necessary for running Galaxy.

5.2.4 Starting Galaxy

While still in the galaxy directory, run the start-up shell script using the command:

```
sh run.sh
```

Note: When run for the first time, this script will take some time to complete.

Subsequent runs will be faster.

Output:

```
Activating virtualenv at .venv
Requirement already satisfied: pip≥8.1 in ./.venv/lib/
→python3.8/site-packages (20.0.2)
...
```

When you see messages like the following in the terminal session, Galaxy is ready to use:

```
Starting server in PID 11466.
serving on http://localhost:8080
```

Leave the terminal window open.

Open a web browser window and type http://localhost:8080 in the address bar.

You will see the home page of your local Galaxy instance (Fig. 85).

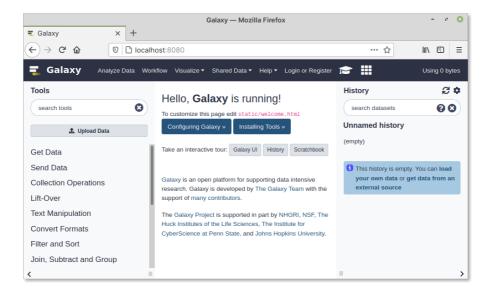


Fig. 85: Home page of your local Galaxy instance

You can start exploring the tools available or even upload data and start using them. However, it is a good idea to *register a user account* now, so you do not lose data, when you clear browser history.

5.2.5 Stopping Galaxy

To stop Galaxy, open the terminal window where you ran the sh run.sh command (Fig. 86).

user@cookbook: ~/programs/galaxy	-	ø	8
File Edit View Search Terminal Help			
127.0.0.1 [06/Apr/2021:06:31:43 +0100] "GET /api/histories/f597429 contents?limit=500&offset=0ℴ=hid&v=dev&q=deleted&q=purged&q=visib e&qv=False&qv=True HTTP/1.1" 200 - "http://localhost:8080/" "Mozilla/5 buntu; Linux x86_64; rv:87.0) Gecko/20100101 Firefox/87.0" [pid: 2438 app: 0 req: 78/93] 127.0.0.1 () {40 vars in 945 bytes} [Tue :31:43 2021] GET /api/histories/f597429621d6eb2b/contents?limit=500&of er=hid&v=dev&q=deleted&q=purged&q=visible&qv=False&qv=False&qv=True => 2 bytes in 174 msecs (HTTP/1.1 200) 3 headers in 139 bytes (1 switche	le&qv .0 () Apr fset= gene	v=Fa (11; 6 :0&o erat	ls U 06 rd ed
0) 127.0.0.1 [06/Apr/2021:06:31:43 +0100] "GET /api/histories/f597429 keys=size%2Cnon_ready_jobs%2Ccontents_active%2Chid_counter HTTP/1.1" 2 ://localhost:8080/" "Mozilla/5.0 (X11; Ubuntu; Linux x86_64; rv:87.0) 0101 Firefox/87.0"	00 -	"ht	tp
<pre>[pid: 2438 app: 0 req: 80/94] 127.0.0.1 () {40 vars in 865 bytes} [Tue :31:43 2021] GET /api/histories/f597429621d6eb2b?keys=size%2Cnon_ready ntents_active%2Chid_counter => generated 112 bytes in 224 msecs (HTTP/ headers in 139 bytes (1 switches on core 1)</pre>	_jobs	%2C	со
127.0.0.1 [06/Apr/2021:06:31:43 +0100] "GET /history/set_as_curren 29621d6eb2b HTTP/1.1" 200 - "http://localhost:8080/" "Mozilla/5.0 (X11 Linux x86_64; rv:87.0) Gecko/20100101 Firefox/87.0" [pid: 2438]app: 0 req: 80/95] 127.0.0.1 () {38 vars in 719 bytes} [Tue	; Ubı Apr	intu 6	; 06
:31:43 2021] GET /history/set_as_current?id=f597429621d6eb2b => genera tes in 278 msecs (HTTP/1.1 200) 7 headers in 207 bytes (1 switches on			^{by}

Fig. 86: Terminal window running Galaxy

Use the Ctrl + c keyboard shortcut to stop Galaxy i.e., press and hold Ctrl key and then press the c key.

When Galaxy has stopped running, you will see a message Finished shutting down (Fig. 87) in the terminal.

user@cookbook: ~/programs/galaxy	-	ø	8
File Edit View Search Terminal Help			
,tN:uWSGIWorker1Core0] Joining monitor thread galaxy.jobs.handler INFO 2021-04-06 06:45:19,184 [pN:main.web.1,p:2438,w: N:uWSGIWorker1Core0] sending stop signal to worker thread			
galaxy.util.monitors DEBUG 2021-04-06 06:45:19,185 [pN:main.web.1,p:2438, ,tN:uWSGIWorker1Core0] Joining monitor thread			
galaxy.jobs.handler INFO 2021-04-06 06:45:19,185 [pN:main.web.1,p:2438,w: N:uWSGIWorker1Core0] job handler queue stopped			
galaxy.jobs.runners INFO 2021-04-06 06:45:19,185 [pN:main.web.1,p:2438,w: N:uWSGIWorker1Core0]_LocalRunner: Sending stop signal to 4 job worker th:	ead:	ls .	
galaxy.jobs.runners INFO 2021-04-06 06:45:19,186 [pN:main.web.1,p:2438,w: N:uWSGIWorker1Core0] Waiting up to 30 seconds for job worker threads to s			
 galaxy.jobs.runners INFO 2021-04-06 06:45:19,186 [pN:main.web.1,p:2438,w: N:uWSGIWorker1Core0] All job worker threads shutdown cleanly	1,m	1:0,	,t
galaxy.jobs.handler INFO 2021-04-06 06:45:19,186 [pN:main.web.1,p:2438,w: N:uWSGIWorker1Core0] sending stop signal to worker thread	1,m	1:0,	t
galaxy.util.monitors DEBUG 2021-04-06 06:45:19,186 [pN:main.web.1,p:2438, ,tN:uWSGIWorker1Core0] Joining monitor thread			
galaxy.jobs.handler INFO 2021-04-06 06:45:19,187 [pN:main.web.1,p:2438,w: N:uWSGIWorker1Core0] job handler stop queue stopped			
galaxy.app DEBUG 2021-04-06 06:45:19,187 [pN:main.web.1,p:2438,w:1,m:0,tM orker1Core0] Finished shutting down	:uW	ISG]	CW .
user@cookbook:~/programs/galaxy\$			

Fig. 87: Galaxy has finished shutting down

You can now close the terminal window.

5.3 Registering a user account

On the Galaxy home page, click on the Login or Register link in the navigation bar (Fig. 88).

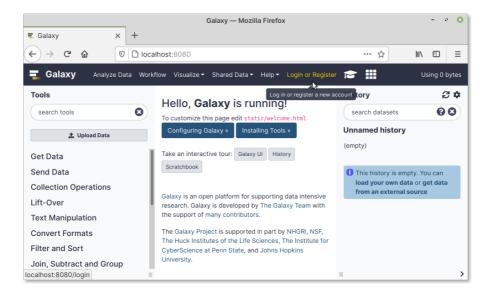


Fig. 88: Click on the Login or Register link

You will be taken to the login page.

Click on the Register here link at the bottom of the page (Fig. 89).

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🗧 Galaxy	Analyze Data Workflow Visualize - Shared Data - Help - Login or Register 🞓 🏢	Using 0 bytes							
	Welcome to Galaxy, please log in								
	Public Name or Email Address								
	Password								
	Forgot password? Click here to reset your password.								
	Login								
	Don't have an account? Register here.								
javascript:void(0)									

Fig. 89: Click on the Register here link

On the Create a Galaxy account page, type in your email address, a password and its confirmation, and a public name (Fig. 90).

Note: This user account is not related to your accounts on usegalaxy.org or other Galaxy servers.

It exists only in your local instance of Galaxy. You can also ignore the notice at the top of the page, which does not apply to local instances.

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← → C ⁴	û 🔽 localhost:8080/login … ☆	III\ □ =					
💶 Galaxy	Analyze Data Workflow Visualize - Shared Data - Help - Login or Register 🞓 🏢	Using 0 bytes					
	Please register only one account - we provide this service free of charge and have limited computational resources. Multi-accounts are tracked and will be subjected to account termination and data deletion.						
	Create a Galaxy account						
	Email Address						
	user@example.org						
	Password						
	•••••						
	Confirm password						
	••••••						
	Public name						
	user						
	Your public name is an identifier that will be used to generate addresses for information you share publicly. Public names mus be at least three characters in length and contain only lower-case letters, numbers, dots, underscores, and dashes ('', '_', '-').						
javascript:void(0)	Create						

Fig. 90: User account creation page

Click on the Create button to proceed.

If account creation was successful, you will be logged in and redirected to the home page of your Galaxy instance.

5.3.1 Managing your account

You can manage your account by clicking on your username in the navigation bar (Fig. 91).

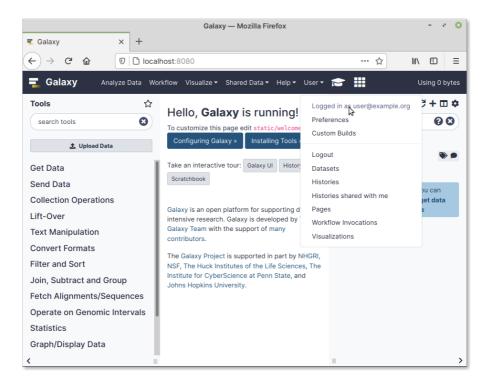


Fig. 91: Logged in as user

If you will be installing additional tools from Galaxy tool shed, this user account will need administrator privileges. You can configure that in the *next step*.

5.4 Granting admin privileges for user

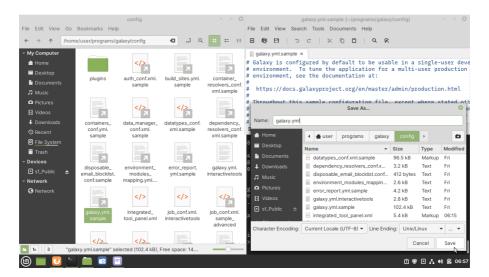
To grant administrator privileges for a user, you will need to create a configuration file for Galaxy and add the user's email address to the list of administrators, and then restart Galaxy for changes to take effect.

5.4.1 Creating a configuration file

A sample configuration file — galaxy.yml.sample, is included with Galaxy.

To create a configuration file using the sample file as template, follow the steps below (see Fig. 92):

- Navigate to the \$HOME/programs/galaxy/config directory using Files
- 2. *Double-click* on galaxy.yml.sample to open it in Text Editor



3. Save it as galaxy.yml in the same directory

Fig. 92: Copying sample configuration file of Galaxy

Note: Alternatively, you can use the *cp* command in a terminal to copy the file.

Assuming you are in the \$HOME/programs/galaxy directory, do:

cp config/galaxy.yml.sample config/galaxy.yml

5.4.2 Adding user to list of admin users

With galaxy.yml open in Text Editor, search for the admin_users setting.

You will find the following section:

```
# Administrative users - set this to a comma-separated
# list of valid Galaxy users (email addresses). These
# users will have access to the Admin section of the
# server, and will have access to create users,
# groups, roles, libraries, and more. For more
# information, see: https://galaxyproject.org/admin/
#admin_users: null
```

Uncomment admin_users by removing the # symbol at the beginning.

Replace null with the email address of the user account.

For example:

admin_users: user@example.org

Save the file.

5.4.3 Restarting Galaxy

Stop Galaxy, if it is running and then start it again.

5.4.4 Verifying admin access

When you log in again, you will see an Admin link in the navigation bar (Fig. 93).

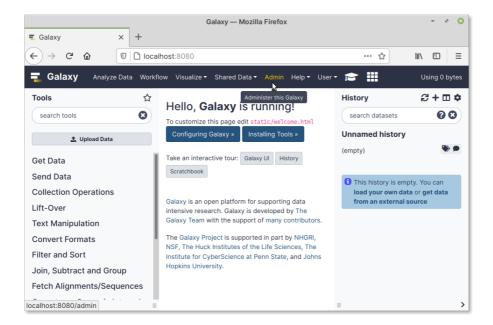


Fig. 93: Admin link in navigation bar

If you click on Admin, you will be taken to the administration page (Fig. 94).

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← → ♂ ŵ < □ □	localhost:8080/admin	···· ☆ II\ 🗉 😑		
Galaxy Analyze Data V	Vorkflow Visualize ▼ Shared Data ▼ Admin Help ▼ User	🕶 💼 Using 0 bytes		
Galaxy version 21.01	Administration			
Server	Please visit the Galaxy administration hub to learn how	to keep your Galaxy in best shape.		
Data Types	Server			
Data Tables	Data Types - See all datatypes available in this 0			
Display Applications	 Data Tables - See all data tables available in this Display Applications - See all display application 			
Jobs	 Jobs - Display all jobs that are currently not finis 			
Workflow Invocations	queued, or running). Administrators are able to c	· · · · · ·		
Local Data	Local Data - Manage the reference (and other) data that is stored within Tool Data Tables. See wiki for details.			
User Management	User Management			
Users	User Management			
Groups	 Users - The primary user management interface with each user and providing operations for rese 			
Roles	information, impersonating a user, and more.	ang pasarisias, apading user		
Forms	Quotas - Manage user space quotas. See wiki for details. Groups - A view of all groups along with the members of the group and the roles			
Tool Management	associated with each group.			
Install and Uninstall	Roles - A view of all non-private roles along with			
	groups that are associated, with the role. Also in datasets that are associated with the role and th			

Fig. 94: Galaxy administration page

Installing tools

To install new tools, click on the following link:

Tool Management \rightarrow Install and Uninstall

You will be taken to the tool management page (Fig. 95).

			Galaxy — M	ozilla Firefox		- 0
🐔 Galaxy	×	+				
← → ♂ ✿		🗅 localhos	st:8080/admin/toolshe	d	☆	III\ 🗊 🗄
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Galaxy version 21.01			Search Repositories			×
Server						
Data Types			Search All O Insta	alled Only		
Data Tables			6230 repositories availa	able at https://toolshed.g2.bx.p	osu.edu/	
Display Applications			Cotomony	Description		Repositories ¢
Jobs			Category	= Description		Repositories 👳
Workflow Invocations			Assembly	Tools for working with asse	mblies	161
Local Data						
User Management			ChIP-seq	Tools for analyzing and ma seg data.	nipulating ChIP-	75
Users						
Groups			Climate Analysis	Tools for analyzing climate	data	5
Roles			Combinatorial	Tools for combinatorial sele		
Forms			Combinatorial Selections	loois for combinatorial sele	ection	9
Tool Management						
	\$		Computational chemistry	Tools for use in computatio	nal chemistry	161
ocalhost:8080/admin/tool	Ished					

Fig. 95: Tool management page

From here, you can search and install tools from the Galaxy main tool shed.

Documentation

Installing and software for managing references and bibliographies, taking notes etc.,

6.1 Managing references using Zotero

Zotero is a free and open-source software for collecting and organizing scientific research articles and other publications.

Articles can be organized using collections and tags, and can be included as citations in the documents you create.

6.1.1 Installing Zotero

You can search and install Zotero using Software Manager.

To save articles from the web and to insert citations in documents, additional add-ons (or extensions) are necessary. You can follow the steps below to install them.

6.1.2 Collecting references from the web

To collect references using a web browser, you will need to install **Zotero Connector** — a browser add-on.

Installing Zotero Connector

To install Zotero Connector in Firefox:

1. Open Zotero from applications menu.

A browser window will open, and you will be taken to the add-on installation page³⁴.

Click on the Install button (Fig. 96).

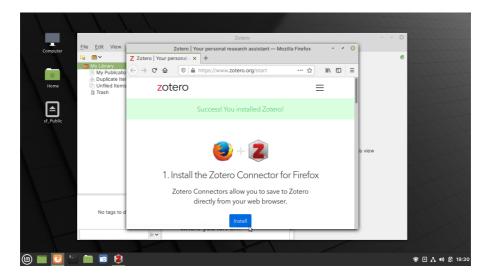


Fig. 96: Zotero add-on installation page

2. You will now see a dialog requesting if you would like to

³⁴ https://www.zotero.org/start

continue installing this add-on from www.zotero.org.

Click on the Continue to Installation button to proceed (Fig. 97).

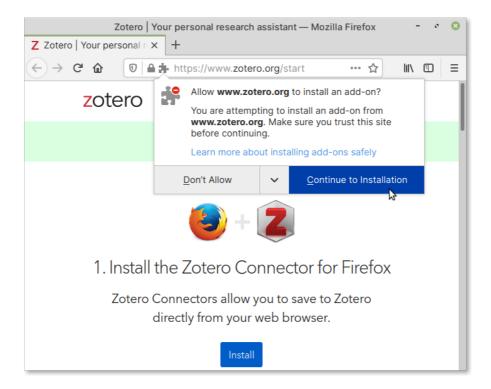


Fig. 97: Click Continue to Installation to proceed

3. You will now see a dialog with information on the permissions required by this add-on.

Click on the Add button to proceed (Fig. 98).

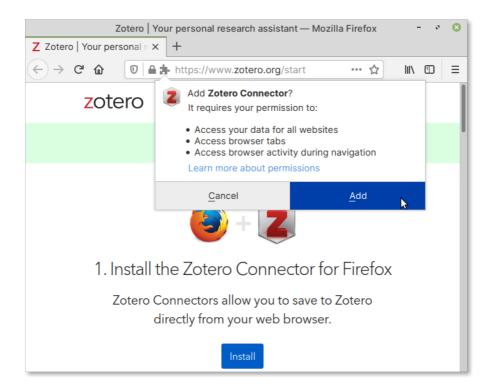


Fig. 98: Click on the Add button to confirm installation

Installation will now proceed.

When complete, you will see a Zotero icon in the browser toolbar (Fig. 99).

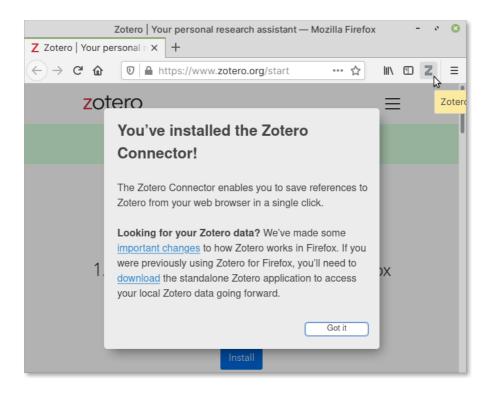


Fig. 99: Zotero Connector installed successfully

You can now start saving articles from the browser to your Zotero library.

6.1.3 Integrating Zotero in LibreOffice

To be able to insert citations and bibliography in your documents, you will need to install the Word Processor Add-in.

Installing Word Processor add-in

To install the add-in in LibreOffice:

1. From the main menu bar of Zotero, select

 $\mathsf{Edit} \to \mathsf{Preferences} \ (Fig. \ 100).$

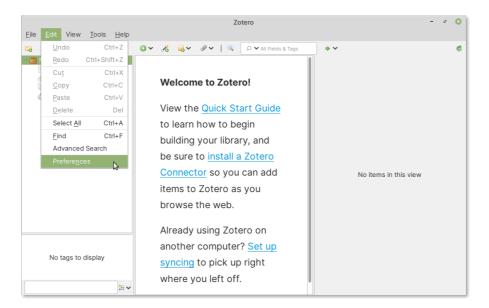


Fig. 100: Viewing Zotero preferences

2. In the Zotero Preferences dialog window that opens, click on the Cite tab.

Now, click on the Word Processors tab to select it.

Click on the Install LibreOffice Add-in button (Fig. 101).

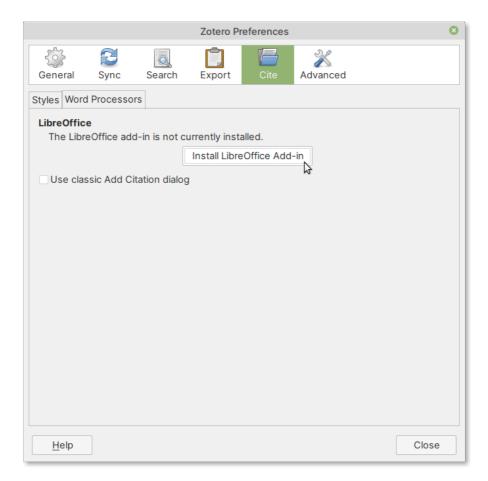


Fig. 101: Installing LibreOffice Add-in from Zotero preferences

3. The Zotero LibreOffice Plugin Installation wizard will now open (Fig. 102)

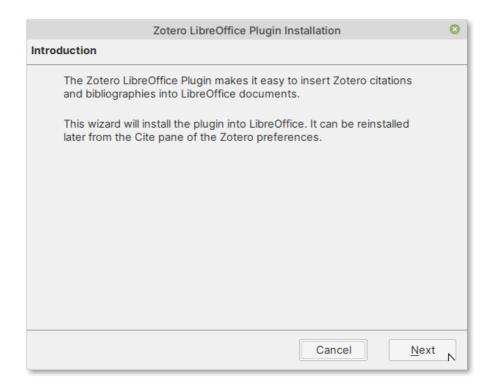


Fig. 102: Zotero LibreOffice Plugin Installation wizard

Click on the Next button to proceed.

4. Click on Manual Installation in the select LibreOffice installations dialog window (Fig. 103).

	Zotero LibreOffice Plugin Installation	8				
Selec	Select LibreOffice unopkg executable					
	Select LibreOffice installations from the list below, or click "Add Installation" to locate the path to an LibreOffice installation directory not shown in the list.					
	To open the directory containing the LibreOffice extension file for manual installation from within LibreOffice, click "Manual Installation".					
Manual Installation Add Directory						
	Cancel <u>B</u> ack <u>N</u> ext					

Fig. 103: Click on the Manual Installation button

A file browser window will open, with the directory set to the location of the add-in file – Zotero_OpenOffice_Integration.oxt (Fig. 104).

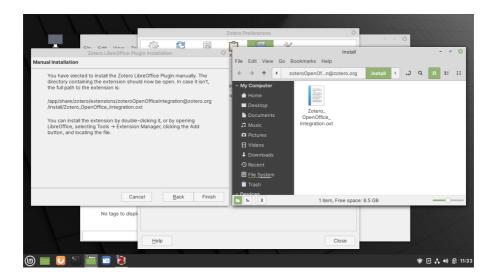


Fig. 104: File browser open with location of the Add-in file

6. *Double-click* on Zotero_OpenOffice_Integration.oxt.

This will open LibreOffice Extension Manager, with a prompt requesting if you would like to install the add-in.

Click on the OK button to confirm (Fig. 105).

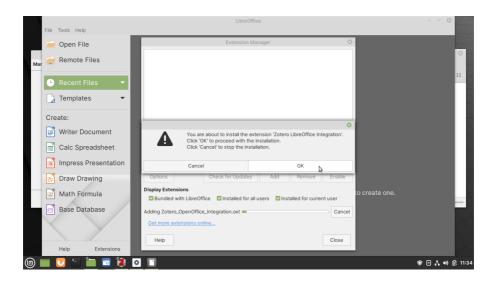


Fig. 105: Click on the OK button in LibreOffice Extension Manager

The add-in will now be installed (Fig. 106).

		Extension Manag	er	8			
*		fice Integrat 5.0.23 Cor ro, an open source researc					
Optior	าร	Check for Updates	Add Remove	Disable			
Display Extensions							
🗹 Bundled with LibreOffice 🛛 🗹 Installed for all users 🖓 Installed for current user							
<u>Get ma</u>	ore extensions on	line					
Help	þ			Close			

Fig. 106: Zotero LibreOffice Add-in installed successfully

If you *restart* LibreOffice, you will notice the Zotero toolbar in the main window (Fig. 107).

Untitled 1 - LibreOffice Writer -	8
File Edit View Insert Format Styles Table Form Tools Window Help	×
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	100%

Fig. 107: Zotero toolbar in LibreOffice

You can now start inserting citations and bibliographies in your documents.

6.2 Creating a notebook using Zim

Zim is a *GUI* application for taking notes on the desktop. You can use it to create and maintain a personal or laboratory notebook on your computer.

6.2.1 Features of Zim

Using Zim, you can:

- **Create digital notebooks** add pages, and organize them using an index page.
- **Take notes quickly** using a WYSIWYG (What You See Is What You Get) interface¹.
- Insert images files, symbols, screenshots, equations and more².
- **Export notes** to formats like HTML, LaTeX, and Markdown.

With the help of plugins, you can add even more functionality.

¹ Similar in functionality to that of word processors like LibreOffice Writer. You do not need to learn a new markup language to use Zim.

² Requires enabling plugins in preferences.

6.2.2 Installing Zim

Zim is available in the distribution repositories.

You can install it using *Software Manager* (Fig. 108).

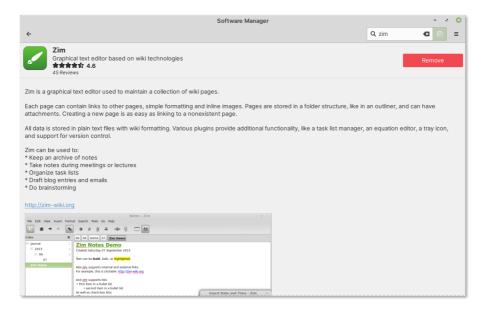


Fig. 108: Installing Zim using Software Manager

6.2.3 Creating a notebook

Open Zim by clicking on its icon in applications menu (Fig. 109). You can use the search bar to locate it quickly.



Fig. 109: Opening Zim from applications menu

When you open the program for the first time, you will notice an Add Notebook dialog (Fig. 110).

Here, you can set a name for this notebook and select a directory to save notebooks.

	Add Notebook	8		
Please se				
Name:	Notes			
Folder:	~/Notebooks/Notes	Browse		
 To create a new notebook you need to select an empty folder. Of course you can also select an existing zim notebook folder. 				
	Cancel	ОК		

Fig. 110: Add notebook

You can accept the defaults.

Click on the OK button to proceed.

This will open the main window of the program (Fig. 111).

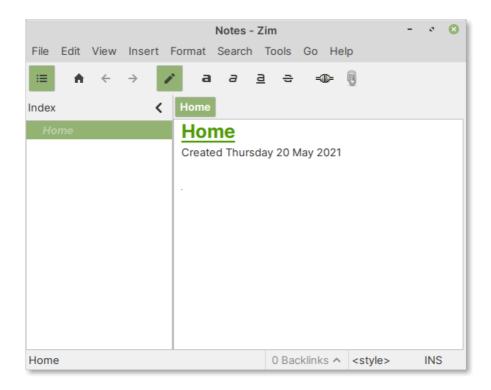


Fig. 111: Main window of Zim

6.2.4 Taking notes

The Home page is the main page of a notebook.

You can start typing your notes here. Zim saves changes automatically.

Basic text formatting

Formatting text in Zim is similar to that of word processor programs.

You can use the Format menu bar entry and select the desired option (Fig. 112).

					Notes - 2	Zim				-	ø	8
File	Edit	View	Insert	Format	Search	Tools	Go	Help)			
:=	A	~	\rightarrow	Head	ing 1		С	trl+1	9			
Index				Head	ing 2		C	trl+2				
			``	Head	ing 3		C	trl+3				
Но	me			Head	ing 4		Ct	trl+4				
				Head	ing 5		Ct	trl+5				
				Bullet	List				ook cre	ated u	sing	
				Numb	pered List							
				Chec	kbox List							
				a Stron	g		Ct	rl+B				
				a Emph	asis		C	trl+l				
				a Mark			Ct	rl+U				
				금 Strike			Ct	rl+K				
				Verba	atim		C	trl+T				
Home	9			Subs	cript	Sh	ift+Ct	rl+B	None		INS	

Fig. 112: Options for formatting text

Keyboard shortcuts

Alternatively, you can use keyboard shortcuts to apply formatting to your text.

For example:

Bold: Ctrl + b

Italic or Emphasis : Ctrl + i

Superscript : Ctrl + Shift + p

Subscript:Ctrl + Shift + b

For headings, use:

Heading 2: Ctrl + 2

Heading 1: Ctrl + 1

Heading 3: Ctrl + 3

Heading 4: Ctrl + 4

Heading 5: Ctrl + 5

Inserting images

To insert an image, you can select the following option from the menu bar:

 $\mathsf{Insert} \to \mathsf{Image}$

In the dialog that opens, browse to the directory containing your image and then select the image (Fig. 113).

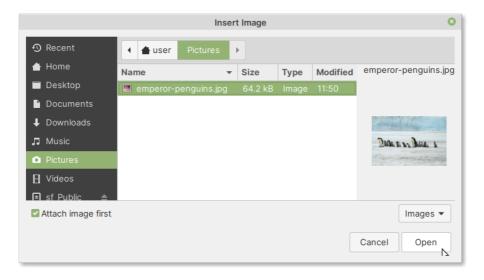


Fig. 113: Insert image. Check Attach image first option

Check the Attach image first option. This will copy the image to your notebook directory.

Click on the Open button to insert the image (Fig. 114).

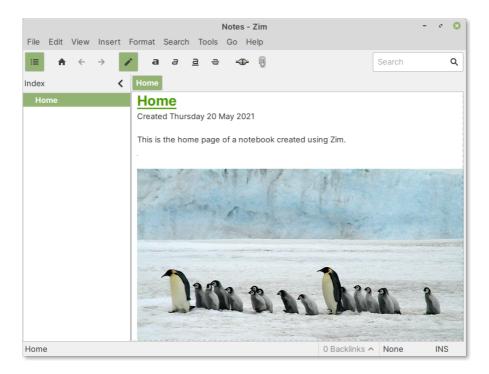


Fig. 114: Image inserted into current page

Resizing an image

If you would like to resize the image, *right-click* on the image and select Edit Properties (Fig. 115).

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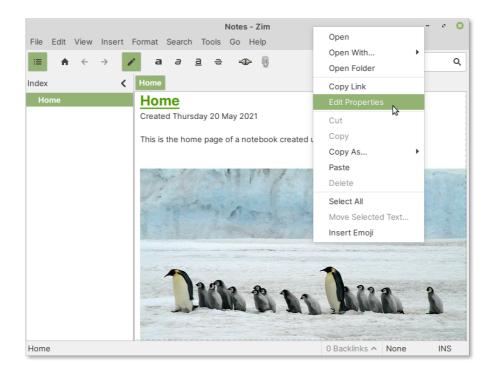


Fig. 115: Edit image properties

In the dialog window that opens, change either the Width or the Height of the image to the desired size and click on the OK button (Fig. 116).

Edit Image				
Location:	mperor-per	nguins	s.jpg	Browse
Link to:				Browse
Width:	500	-	+	
Height:	332	-	+	
				Reset Size
		Can	cel	ок

Fig. 116: Change the width or height of the image

The image will now be resized (Fig. 117).

Linux for Biologists

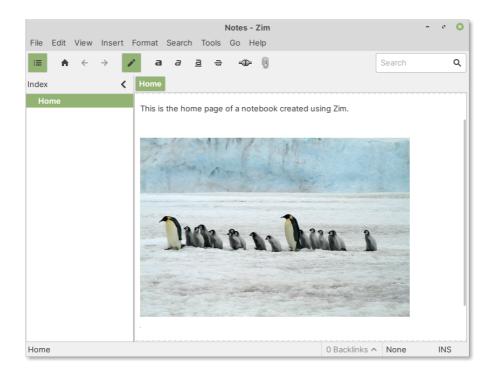


Fig. 117: Resized image

Adding more pages

To add more pages, select the following option from the menu bar (Fig. 118):

 $\mathbf{File} \rightarrow \mathbf{New} \ \mathbf{Page}$

Note: You can also *right-click* on a page in the Index view and select the New Page Here option.

	Notes - Zim	- * 😢
File Edit View Insert Format Search	Tools Go Help	
New Page 📐 Ctrl+N	a -0- N	Search Q
New Sub Page Shift+Ctrl+N		
Open Another Notebook Ctrl+O	e 2 Home	
Import Page	ALL C IT ALL	1
Save Version Shift+Ctrl+S		
Versions		- mar
Open in New Window	and the second of the second of	and the second sec
Save Ctrl+S	And the second	
Save A Copy		
Export		
Send To		
Print to Browser Ctrl+P		
Rename Page F2		
Move Page		
Delete Page		
Properties		
Close Ctrl+W		
Quit Ctrl+Q	0 Backlin	ks 🔨 <style> INS</th></tr></tbody></table></style>

Fig. 118: Adding a new page

Enter a name for the page in the New Page dialog window (Fig. 119) and click on the OK button.

New Page 😣				
 Please note that linking to a non-existing page also creates a new page automatically. 				
Page Name:	Useful Links			
Page Template:	Default 👻			
Help	Cancel OK	27		

Fig. 119: Enter a name for the new page

The new page will appear in the Index view (Fig. 120).

	Notes - Zim		-	ø 🙁
File Edit View Insert F	Format Search Tools Go Help			
Index ← →			Search	٩
Home Useful Links	Useful Links Created Saturday 22 May 2021			
	6			
Useful Links		0 Backlinks 🔨	None	INS

Fig. 120: Newly added page

Adding subpages

A subpage will be placed under an *existing* page.

To add a new subpage:

- 1. Select an existing page in Index view
- 2. Select $\mathsf{File} \to \mathsf{New} \operatorname{\mathsf{Sub}} \mathsf{Page}$ from the menu bar
- 3. Enter a name for the page and click on the OK button

Deleting or renaming pages

To delete or rename pages, you can *right-click* on the page and select the desired function.

6.2.5 Exporting notes and notebooks

To export the notebook or a page, select:

 $\mathsf{File} \to \mathsf{Export}$

In the dialog window that appears, select the desired option and click on the Forward button (Fig. 121).

		Exp	ort	8	
Select t	he pag	es to export		(1/3)	
 Com 	plete n	otebook			
OSing	le page				
Page:	Page: :Home				
🗹 Inclu	ide sub	pages			
Hel	p	Cancel	Back	Forward	

Fig. 121: Export notebook

In the next screen, you can select the format of the exported notebook or page in the Format drop-down box (Fig. 122).

	Export	8	
Select the e	Select the export format		
Format:	HTML		
Template:	MHTML (Web Page Archive)		
	LaTeX	Browse	
	Markdown (pandoc)		
O Link files	RST (sphinx)	path	
Map doc	ument root to URL:		
	Get more templates online		
Help	Cancel Back	Forward	

Fig. 122: Select an export format

You can leave it at the default — HTML. Click on the Forward button to proceed.

In the final screen, select a directory to save the exported notebook or page.

Note: If you are using the defaults, it is a good idea to create a new output directory and select it under **Output folder**.

Click on the OK button complete export.

	Export	8	
Select the output file or folder			
Export each Export all page			
Output folder:	~/Documents/zim-export	Browse	
Index page:			
Help	Cancel Back	ок	

Fig. 123: Select an output folder

When complete, open the output directory in file manager.

Double-click on Home.html to open it in the browser (Fig. 124).

Linux for Biologists

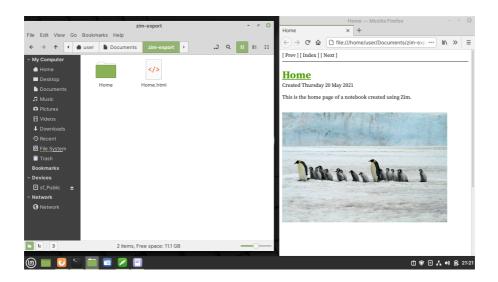


Fig. 124: Viewing exported notebook

6.2.6 Activating more features using plugins

These are some plugins included with Zim:

Insert Symbol – insert special symbols and characters

- **Table of Contents** adds a widget displaying the current page's table of contents
- **Tags** add tags to your notes
- **Tray Icon** adds an icon to system tray for quick access to your notebooks
- **Spell Checker** adds support for checking spelling

_

You will need to activate (or enable) them in preferences, before you can start using them.

Enabling a plugin

To enable a plugin:

- 1. Select $Edit \rightarrow Preferences$
- 2. Click on the Plugins tab
- 3. Check the box corresponding to the plugin you wish to enable (Fig. 125)
- 4. Click on the OK button

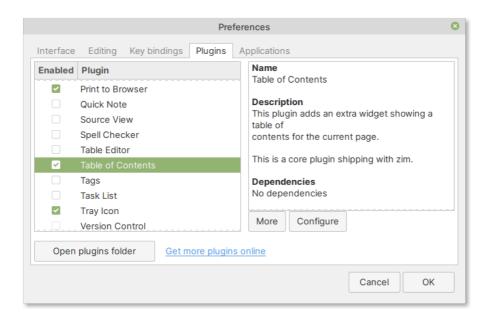


Fig. 125: Enabling plugins

Note: Some plugins have additional options.

Click on the **Configure** button below the plugin description to access these options.

6.2.7 Getting help

Zim includes a detailed user manual. You can access this by selecting (Fig. 126):

$\mathsf{Help} \to \mathsf{Contents}$

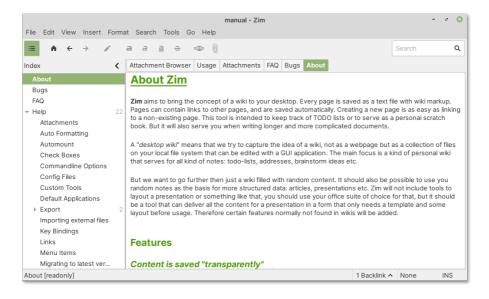


Fig. 126: Help on using Zim

Glossary

Anaconda A free and open-source (Anaconda Individual Edition) Python and R distribution. It includes *Conda* and more than 250 open-source scientific packages. Additional packages can be installed from *Anaconda Cloud* repositories.

Website: https://www.anaconda.com/products/individual

Anaconda Cloud Repository for Python and R packages and notebooks.

Website: https://anaconda.org

apt A command-line program that handles the installation and removal of software on Debian, Ubuntu and other Linux distributions.

Related section:

-> The command-line version (apt)

bioconda A channel for *Conda* package manager with over 7000

packages of bioinformatics software.

Website: https://bioconda.github.io/

- **build-essential** A package that installs software build tools like make and compilers like gcc, which are required for build-ing modules written in languages like C.
- **Bash** *GNU* project's shell program. The name stands for The Bourne-Again Shell. It is the most commonly used shell in Linux distributions.

Website: https://www.gnu.org/software/bash/

Bioconductor Tools written in the R programming language for the analysis and comprehension of high-throughput genomic data.

Website: https://www.bioconductor.org/

BiocManager An R package to install and update packages from the *Bioconductor* project repository.

Website: https://cran.r-project.org/package= BiocManager

BioPython Python tools for computational molecular biology.

Website: http://biopython.org/

Bio::Phylo Perl package for phylogenetic analysis.

Website: https://metacpan.org/pod/Bio::Phylo

commands Also called as binaries or executables.

Conda Conda is a package and environment manager.

As a *package manager*, it can be used to install software from *Anaconda Cloud*. Software *dependencies* will be installed automatically.

As an *environment manager*, it can be used to create and manage environments containing different sets of packages. You can activate and use these environments as necessary.

cpanminus A Perl script to get, build and install modules from *CPAN*. It provides the cpanm command.

Website: https://metacpan.org/pod/App::cpanminus

cutadapt A Python program that finds and removes adapter sequences, primers, poly-A tails and other unwanted sequences from high-throughput sequencing reads.

Website: https://cutadapt.readthedocs.io

CPAN Abbreviation for Comprehensive Perl Archive Network. It provides additional Perl modules for installation (196,752 as of Dec 2020).

Website: https://www.cpan.org/

CRAN Abbreviation for Comprehensive R Archive Network. A network of FTP and web servers providing up-to-date versions of R, packages and documentation.

Website: https://cran.r-project.org/

Debian A Linux distribution made of free and open source software. It is free for anyone to download, use, modify and distribute.

Website: https://www.debian.org/

- **Debian package** An archive of executable files, libraries, and documentation of software. It can be installed on Debian Linux and Debian-based systems like Ubuntu and Linux Mint. These files have the .deb file extension.
- **dependencies** Additional programs or libraries that are needed for a program to work.
- **edgeR** An R package for empirical analysis of digital gene expression data. It is available from the *Bioconductor* project repository.

Website: https://www.bioconductor.org/packages/edgeR/

FAST Abbreviation for FAST Analysis of Sequences Toolbox. A set of utilities written in Perl that extend the UNIX paradigm to bioinformatic sequence records.

Website: https://metacpan.org/pod/FAST

- **Files** The default file manager in *Linux Mint* Cinnamon edition. Its original name is Nemo.
- **gdebi** A simple tool to install *Debian package* files along with their *dependencies* (if any).

Website: https://launchpad.net/gdebi

GNU GNU is a recursive acronym for GNU's Not Unix. The goal of the project is to offer a Unix-compatible system that would be 100% free software.

Website: https://www.gnu.org/

- **GUI** Abbreviation for graphical user interface. On a personal computer, it typically includes application windows with buttons to access their functions, icons for launching applications and widgets for managing devices and services.
- **IDE** Abbreviation for integrated development environment. Some examples include PyCharm, RStudio and Eclipse.
- **local-lib** A Perl module to create a local directory structure to install modules with their *dependencies* without requiring administrator privileges.

Website: https://metacpan.org/pod/local::lib

Linux Mint A desktop Linux distribution. It is based on *Debian* and *Ubuntu*.

Website: https://linuxmint.com/

MEGA Software for Molecular Evolutionary Genetics Analysis. Available as *GUI* and command-line versions.

Website: https://megasoftware.net/

MetaCPAN A search engine for Perl packages and modules available on *CPAN*.

Website: https://metacpan.org/

Miniconda A minimal distribution of *Conda*. It is faster to install and also uses less disk space, when compared to *Anaconda* — the alternative installer which comes bundled with additional packages.

Website: https://docs.conda.io/en/latest/miniconda.html

Modeller A program for comparative protein structure modelling by satisfaction of spatial restraints.

Website: https://salilab.org/modeller/

nano A simple command-line based text editor.

Website: https://www.nano-editor.org/

- **OVA** A file format for distributing virtual machine images.
- **pip** The Python package installer. It can be used to install packages from *PyPI* and other Python package indexes.

Website: https://pip.pypa.io/

PyMOL PyMOL is a molecular visualization system originally developed by Warren L. Delano. It is currently maintained by Schrödinger, Inc.

Website: https://pymol.org/2/

PyPI Abbreviation for Python Package Index. Repository for software written in Python (275,161 projects as of Dec 2020).

Website: https://pypi.org/

- root The primary administrator account on a Linux system.
- **R** Programming language and free software environment for statistical computing and graphics.

Website: https://r-project.org

RStudio Desktop An *IDE* for *R*. It includes an R console, an editor with syntax-highlighting and tools for plotting, debug-

ging and managing R packages. The open-source version can be downloaded for free from the project website.

Website: https://rstudio.com/products/rstudio/download/

Related sections:

-> Installing a Debian package

- **setuptools** Python program for building and installing Python packages.
- **shell** The shell provides a command-line interface (CLI) to the operating system's services.
- **Software Manager** The default application(*GUI*), for installing software on Linux Mint.

Applications with similar functionality are available on other Linux distributions. For example:

- Ubuntu Software on Ubuntu
- Software on Fedora and other GNOME-based distributions
- Discover on Kubuntu and other KDE-based distributions.

Related sections:

-> The quick and easy method

Synaptic A GUI package manager for systems using apt.

Website: https://www.nongnu.org/synaptic/

text editor Program to edit text files.

Examples (*GUI*) - Text Editor (xed) on Linux Mint, Text Editor (gedit) on Ubuntu, Kwrite on KDE Plasma, Geany etc.,

Examples (command-line) — *nano*, VIM or vi, GNU Emacs etc.,

Related sections:

-> Text Editor — create and edit text files

-> Editing text files using nano

Ubuntu Linux distribution developed by Canonical and community of developers. It is based on *Debian*.

Website: https://ubuntu.com/

wheel Python program for installing packages distributed in Python wheel (.whl) format.

Credits

This book is created on a Linux system using open source software. Fonts and images used are under an open source licence or in the public domain.

Software

Linux Mint – https://linuxmint.com	
Sphinx – https://www.sphinx-doc.org	g/en/master/
sphinx-autobuild extension — executablebooks/sphinx-autobuil	https://github.com/ ld
LaTeX for generating PDF - https://ww	ww.latex-project.org/
GNOME Builder for editing text – Apps/Builder	https://wiki.gnome.org/
Firefox for previewing HTML – H en-GB/firefox/	https://www.mozilla.org/
Pandoc for converting HTML to ODT	— https://pandoc.org/

LibreOffice for proofreading – https://www.libreoffice.org/

LanguageTool extension for spelling and grammar checks – https://languagetool.org/

Inkscape for editing images - https://inkscape.org/

GIMP for editing images – https://www.gimp.org/

Building and testing the virtual machine

Ansible – https://www.ansible.com/

Vagrant – https://www.vagrantup.com/

VirtualBox – https://www.virtualbox.org/

Fonts

Source Serif 4 – https://github.com/adobe-fonts/source-serif/

Fira Sans – https://github.com/mozilla/Fira

Fira Code – https://github.com/tonsky/FiraCode

Recursive Mono – https://github.com/arrowtype/recursive

Images

The emperor penguin image used in the book cover, is obtained from openclipart.org.

https://openclipart.org/detail/47299/emperor-penguin

genindex

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