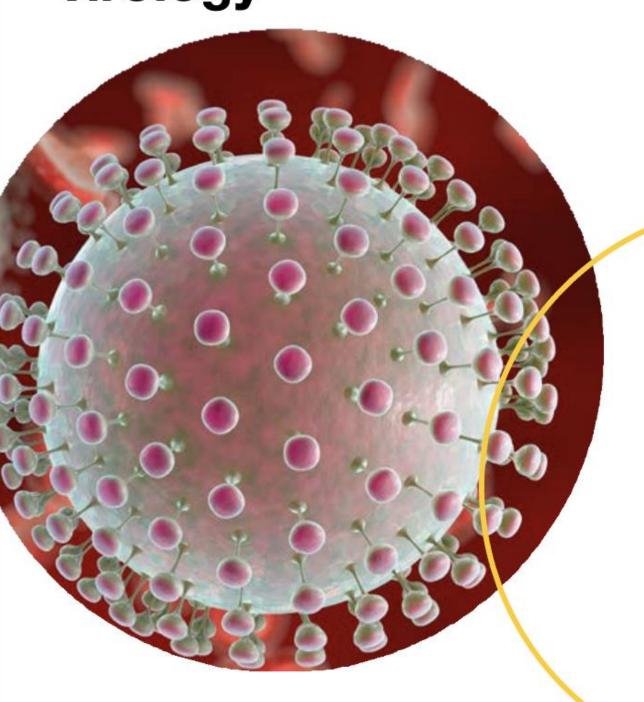


# genomics and clinical virology 18-23 February 2024



Informatics Course Guide



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# **Informatics Guide About**

The Informatics Guide is your go-to resource after completing the course. It not only guides you through downloading course materials on GitHub, setting up virtual machines, and installing software used in the course but also serves as a roadmap for your journey. Additionally, each section concludes with hyperlinks to extra resources that will help you with troubleshooting. Happy learning!

# **Course Resources on GitHub**

Our course materials, including slides, files, and essential information, have been conveniently hosted on our dedicated GitHub repository. The material shared has been licensed under a <a href="https://example.com/BY-NC-SA">BY-NC-SA</a>, <a href="https://example.com/Attribution-NonCommercial-ShareAlike 4.0 International (CC BY-NC-SA 4.0">Attribution-NonCommercial-ShareAlike 4.0 International (CC BY-NC-SA 4.0)</a> and will be available for indefinitely.

Check out your course GitHub Page at <a href="https://github.com/WCSCourses/GCV24">https://github.com/WCSCourses/GCV24</a>.

# Accessing the Virtual Machine (VM) image via Globus

Virtual Box is a cross-platform application developed by Oracle which enables you to create Virtual Machines (VMs). To streamline your learning experience, we offer access to a pre-configured virtual machine through Globus. This virtual machine comes equipped with all the necessary software used throughout the course. By downloading this VM file, you can quickly dive into the practical aspects of informatics without the hassle of individually installing software components.

# **Virtual Machine Setup Guides**

For users on macOS and Windows operating systems, we provide comprehensive setup guides to help you configure the virtual machine. These step-by-step guides are designed to ensure a seamless setup process, allowing you to focus on learning rather than troubleshooting technical issues.

# **Software Installation Details**

In addition to the virtual machine option, we understand that some users may prefer to install software directly on their laptops. That's why we've included detailed software installation instructions for all tools covered in the course.



# GitHub and how to make most out of it

GitHub is an open source, web-based platform primarily used for version control and collaboration on software development projects. It allows users to store and manage their code, track changes made to files, and coordinate work among team members.

Within GitHub, users organize their content into repositories. A repository, often referred to as "repo," is a collection of files and folders associated with a specific project or application. These files can include source code, documentation, configuration files, and more. Repositories provide a centralized location for storing and managing project-related assets, making it easier for collaborators to access and contribute to the project.

Course materials, such as slides, files, and essential information shared during the course, are typically stored in a dedicated repository on GitHub. This repository serves as a central hub for accessing all the materials related to the course. Users can navigate through the repository's folders to locate specific files or use the search functionality to find relevant content quickly.

As a reminder, access to the Learning Management System (LMS) used during the course will be withdrawn two months post-course. However, the GitHub repository will remain accessible indefinitely, making it an invaluable long-term resource for participants. By bookmarking the repository or saving its URL, participants can continue to access course materials, review content, and engage with the community even after the course has ended.

Check out your course specific GitHub Page at <a href="https://github.com/WCSCourses/GCV24">https://github.com/WCSCourses/GCV24</a>.

If you want to learn more about GitHub and how you can use it in your research, please refer <u>GitHub</u> <u>Docs</u>.

# **Downloading Virtual Machine (VM) image via Globus**

The Virtual Machine (VM) is a huge download that many users have difficulty with. As a result, we will rely on Globus software to help us.

Globus is a research-oriented file transfer software. The main advantage of using globus is that if there is an internet connection failure during downloading, it will stop and resume from the same position instead of resetting to zero percent.

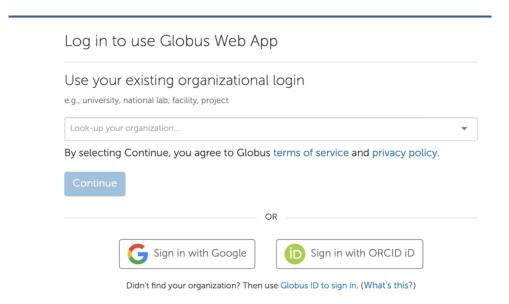
Globus website: https://www.globus.org



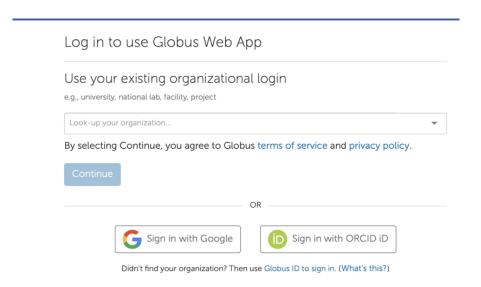
# **Globus VM Downloading Steps:**

1. Make a globus connect personal account by going this webpage, and choose the download for your operating system (Mac or Windows), which will prompt you to make an account: <a href="https://www.globus.org/globus-connect-personal">https://www.globus.org/globus-connect-personal</a>

Choose to use globus ID to sign in (picture below)



Then if you don't have an ID yet, select "Need a Globus ID? Sign up".





Log In with Glob	us ID		Need a Globus ID? Sign Up
		s to your <b>globusid.org</b> acco auth.globus.org. If you app	•
Username			@globusid.org
Password			
	Log In		Forgot password?

Then make sure you specify for research or educational purposes. And create your account. Remember your password for the later steps.

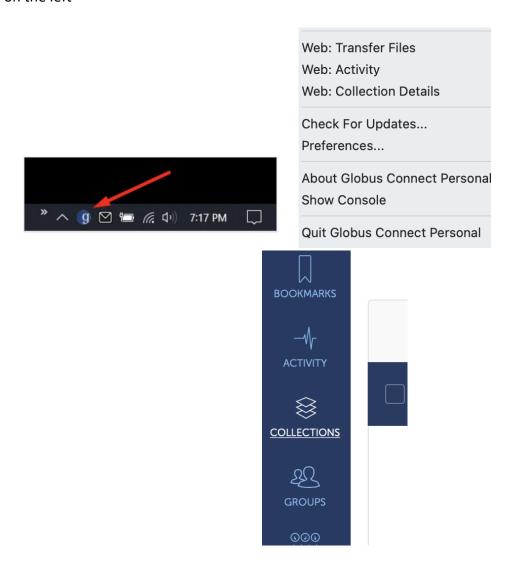
Create a Globus ID	Already have a Globus ID? Log In
	g access to your <b>globusid.org</b> account for accessing a cated at auth.globus.org. If you approve, please create a
Username	@globusid.org
	Your username will be checked for availability.  Usernames may contain both letters and numbers, but must begin with a letter and be between 3 and 31 characters long. NOTE: this is an ID you are creating – not a working e-mail address
Password	
	□ show password
Full Name	first and last name
E-mail	user@example.edu
This account will be used for	onon-profit research or educational purposes
	o commercial purposes
Organization	
	☐ I have read and agree to the Globus Terms of Service and Privacy Policy

2. Then download the globus client onto your local machine (or where you intend to run the VM), allow it to install. It will ask for a collection name; give it a name you will refer to - example



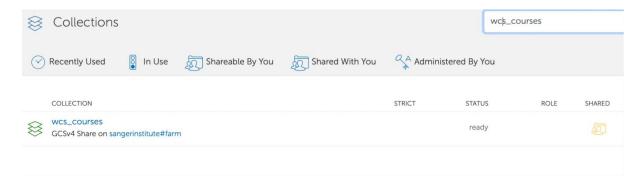
"home\_computer" or "local\_mac". This is a name for the local folders on your computer that we will send the VM to in a later step.

- 3. Click on the small "g" icon on the task bar and select Web: Transfer Files. **Note:** For linux users there may not be a shortcut. Once you start globus personal connect via command line, navigate to <a href="https://app.globus.org/file-manager">https://app.globus.org/file-manager</a> to begin the file manager.
- 4. You will see your own files on this page. Your local endpoint is your computer. Click on "Collections" on the left



5. Search for the endpoint at wcs\_data\_transfers

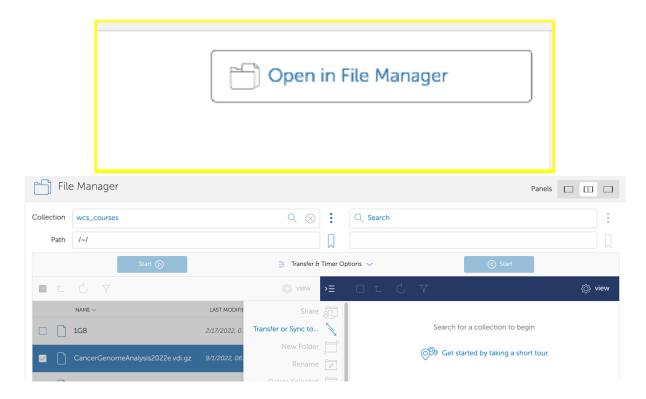




Click on the endpoint labelled wcs data transfers

Then click on "Open in File Manager" will open a file manager

6. Then we begin the steps to transfer the VM to your local machine. First, select the VM file "GCV2024.vdi.gz" with the check box. Then click on "Transfer or sync to".

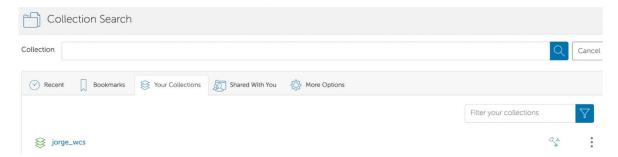


Then click on the search box in the opposite panel

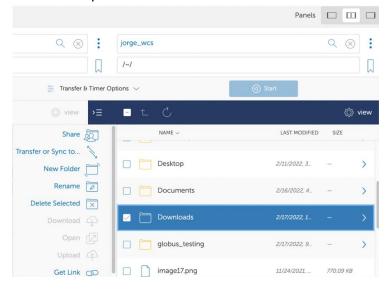
7. Click on "Your Collections" and select your local endpoint (the name will be what you gave it during the globus personal connect installation)

You can also browse to choose the specific directory or folder on your local machine you want the VM to be download in.





Downloads is selected in this example.



- 8. When you have chosen the local location, click on the "Start" button under the "wcs\_data\_transfers" section to begin the download to your local endpoint.
- 9. Wait for download completion it will email you to the account you set up, and you can track the transfer in the "Activity" menu.
- 10. Run the installation of VirtualBox, then install the virtual machine you have just downloaded.

# Additional Resources and Troubleshooting for VM image and Globus

- Globus Documentation: <a href="https://docs.globus.org/guides/">https://docs.globus.org/guides/</a>
- Virtual Box Documentation: <a href="https://www.virtualbox.org/wiki/Documentation">https://www.virtualbox.org/wiki/Documentation</a>
- Virtual Box Manual: https://www.virtualbox.org/manual/ch01.html
- Virtual Box Forum: <a href="https://forums.virtualbox.org/index.php">https://forums.virtualbox.org/index.php</a> (helpful for finding similar problem queries and solutions)
- Stack overflow: https://stackoverflow.com/ (Public Q&A platform for debugging)
- Bioinformatics (BioStars) Forum: <a href="https://www.biostars.org/t/Forum/">https://www.biostars.org/t/Forum/</a> (General Bioinformatics queries)



# Introduction to Virtual Box and Virtual Machine

Virtual Box is a cross-platform application developed by Oracle which enables you to create Virtual Machines (VMs). The VM generates a guest operating system (such as Linux) derived from a host operating system (The host operating system is the primary and foundational operating system that runs directly on the physical hardware of a computer.). Therefore, sufficient RAM, processors, and memory in the host operating system are essential for smooth running of VMs.

Note: The VM image file (.vdi) contains all the software installed for the course.

# **Host OS Requirements for Virtual Box**

RAM requirement: 8GB (preferably 12GB)

Processor requirement: 4 processors (preferably 8)

Hard disk space: 200GB

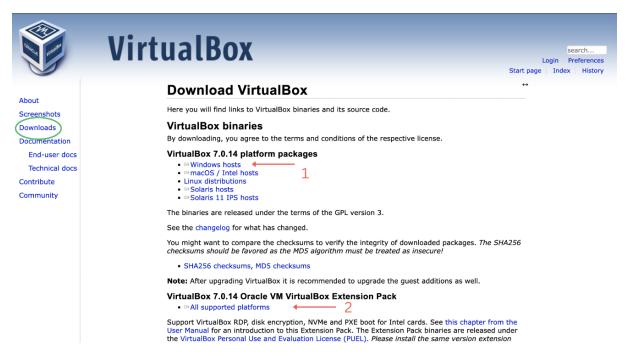
Admin rights to the computer.

**Note:** Please be aware that Virtual Box is currently incompatible with M1/M2/M3 chips on MacBook. It is exclusively designed for use on Intel-based MacBooks. The current version in use is Virtual Box 7.0.

# Installation of Virtual Box for Windows OS

#### 1. Download VirtualBox:

Navigate to the official VirtualBox website (<a href="https://www.virtualbox.org/">https://www.virtualbox.org/</a>) and go to the "Downloads" section. Choose the version that matches your Windows operating system (32-bit or 64-bit).





# 2. Download Extension Pack (Optional):

If needed, download the VirtualBox Extension Pack from the same "Downloads" section. This pack provides additional functionalities like USB 2.0 and 3.0 support, VirtualBox Remote Desktop Protocol (VRDP), and more.

#### 3. Run the Installer:

Locate the downloaded VirtualBox installer file (.exe) and double-click to run it. Follow the on-screen instructions provided by the installer. Click "Next" to proceed through the setup wizard. You may customize installation options if desired.

# 4. Install Extension Pack (Optional):

If you downloaded the Extension Pack, double-click on the file (e.g., Oracle\_VM\_VirtualBox\_Extension\_Pack-6.0.14-133895.vbox-extpack) to install it. This can be done after VirtualBox installation.

# 5. Complete the Installation:

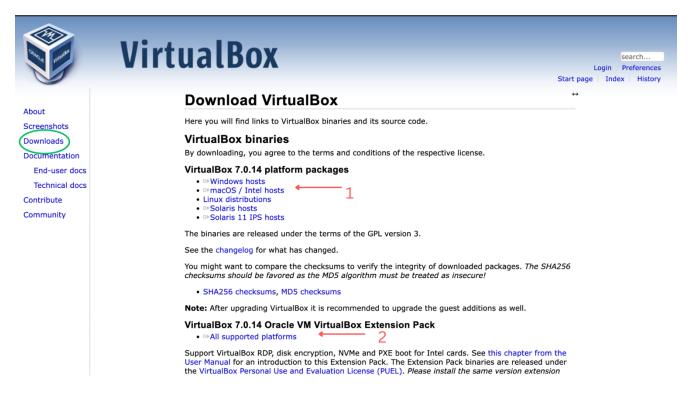
Once the installation is complete, click "Finish" to exit the installer.

# **Installation of Virtual Box for MacOS**

#### 1. Download VirtualBox:

Navigate to the official VirtualBox website (<a href="https://www.virtualbox.org/">https://www.virtualbox.org/</a>) and go to the "Downloads" section. Choose the version compatible with macOS.





### 2. Download Extension Pack (Optional):

If needed, download the VirtualBox Extension Pack from the same "Downloads" section. This pack provides additional functionalities like USB 2.0 and 3.0 support, VirtualBox Remote Desktop Protocol (VRDP), and more.

#### 3. Run the Installer:

Locate the downloaded VirtualBox installer file (.dmg) and double-click to open it. Follow the on-screen instructions to install VirtualBox on your macOS. Drag the VirtualBox icon to the Applications folder.

# 4. Install Extension Pack (Optional):

If you downloaded the Extension Pack, double-click on the file (e.g., Oracle\_VM\_VirtualBox\_Extension\_Pack-6.0.14-133895.vbox-extpack) to install it. This can be done after VirtualBox installation.

### 5. Complete the Installation:

Once installed, open VirtualBox from Applications folder. The first time you run it, macOS may ask for permission to run the application. Click "Open" to proceed.



# Installing a Virtual Machine (VM) image

Virtual Machine image (.vdi extension file) is a replication of the exact VM used during the course. Downloading and installation of the VM image would save you time from installing each software individually and can also find exercise data on the same. If for some reason you are unable to find data it should be available in the <u>course GitHub repository</u>.

**Note:** Although the VM image file (.vdi) contains all the software installed for the course, you still need admin rights of the computer to run some sudo commands.

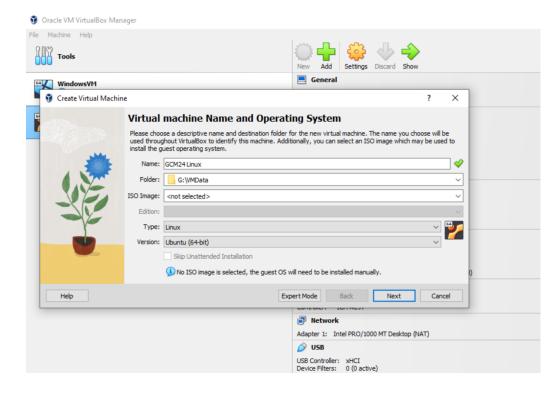
#### 1. Start VirtualBox:

Locate the VirtualBox shortcut on your desktop or find it in the Start Menu. Double-click on the VirtualBox icon to launch the application.

#### 2. Create a Virtual Machine:

In the VirtualBox Manager, click "New" for a new virtual machine. Enter a name for your virtual machine (e.g., "CourseName 2024"). Choose "Linux" as the type and select "Ubuntu 64-bit" as the version. For example, we have taken CourseName as "GCM 24".

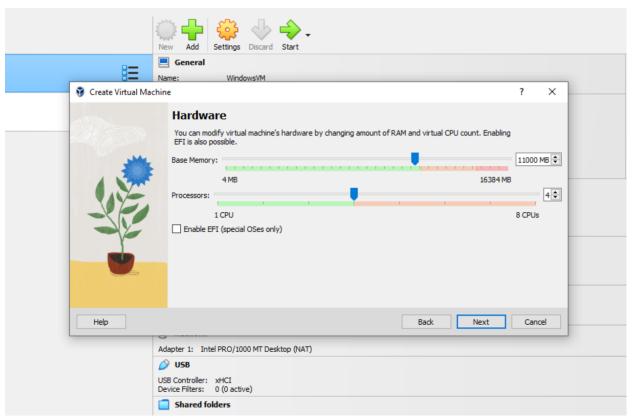
Note: Current Genomics and Clinical Virology course is saved as "GCV2024.vdi"



#### 3. Memory (RAM) Allocation:

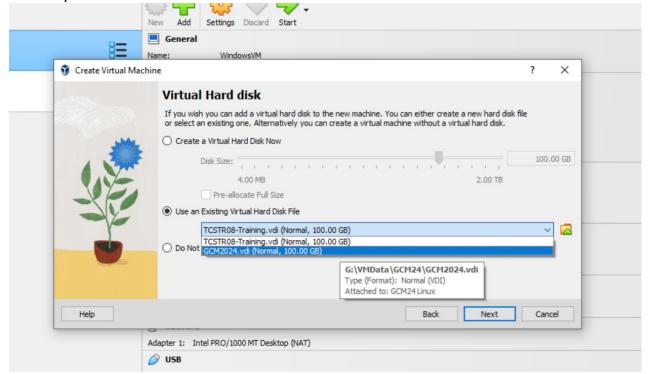
In the window that follows, determine the amount of RAM to allocate, keeping it close to the top of the green section on a PC. Also, adjust the number of processors, ideally half of the available ones. Click Next when settings are configured.





#### 4. Hard Disk:

Indicate the location of the virtual machine file you downloaded. Choose 'Use an existing virtual hard disk file,' click the icon next to the menu, and add the .vdi file. Confirm your selection in the summary window and click Finish.



#### 5. Follow Ubuntu Installation Wizard:

Follow the on-screen instructions to install Ubuntu. Choose language, keyboard layout, and select "Install Ubuntu." Follow the prompts for time zone, user account, and installation type.



# 6. Complete Installation:

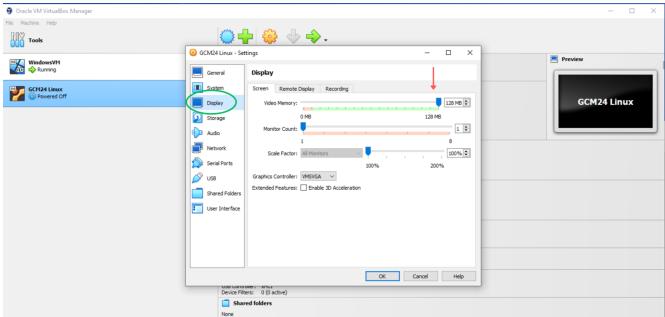
Allow the installation process to complete. Possibly, VM Box might ask you to restart the virtual machine. Double-check your choices in the confirmation window. Once satisfied, start the virtual machine by highlighting its name and clicking the 'Start' icon in the manager window.

### 7. Adjust Screen Size:

The screen resolution should automatically adjust to match your VirtualBox window size. If it doesn't, you can manually adjust the screen size in the Ubuntu VM.

Go to "Settings" > "Displays" in the Ubuntu system settings.

You should see different screen resolutions available. Select the desired resolution that fits your VirtualBox window.



#### 8. Login Ubuntu:

The virtual machine will go through a boot process. After a short time, a window will appear.

**Note:** For this course, the user account is named 'manager,' and the password, if required, is also 'manager'.

# **Running and Managing VMs (Optional)**

Adjusting the screen size in an Ubuntu virtual machine (VM) within VirtualBox involves installing and configuring the VirtualBox Guest Additions. By installing VirtualBox Guest Additions, you enable features like automatic screen resizing, improved graphics performance, and seamless mouse integration between your host machine and the Ubuntu VM. Here are the steps to achieve this:

### 1. Start Ubuntu VM:

Ensure that your Ubuntu VM is running.

#### 2. Insert Guest Additions CD:



In the VirtualBox menu, go to "Devices" and choose "Insert Guest Additions CD image." This action virtually inserts the Guest Additions CD into your Ubuntu VM.

# 3. Open Terminal:

Open a terminal window in Ubuntu. You can do this by pressing 'Ctrl + Alt + T' or using the application launcher.

# 4. Navigate to the CD Directory:

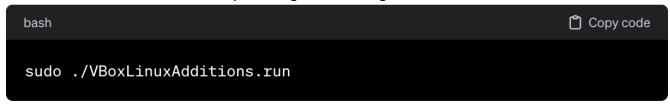
Change to the directory where the Guest Additions CD is mounted. This is often located in the '/media' directory. Use the following command to navigate to the directory:



Note: The directory name may vary based on your VirtualBox version.

# 5. Run Guest Additions Installer:

Run the Guest Additions installer by entering the following command in the terminal:



**Note:** You may be prompted to enter your password.

#### 6. Follow Installation Wizard:

The Guest Additions installer will launch an installation wizard. Follow the prompts to complete the installation.

#### 7. Reboot Ubuntu VM:

After the installation is complete, it's recommended to reboot your Ubuntu VM to apply the changes.

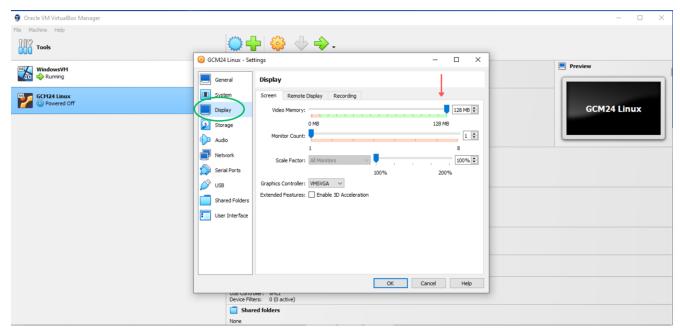
# 8. Adjust Screen Size:

Once the VM has restarted, the screen resolution should automatically adjust to match your VirtualBox window size. If it doesn't, you can manually adjust the screen size in the Ubuntu VM.

Go to "Settings" > "Displays" in the Ubuntu system settings.

You should see different screen resolutions available. Select the desired resolution that fits your VirtualBox window.





# 9. Verify Changes:

Confirm that the screen resolution has changed and suits your preferences.

### 10. Manage VM Settings:

In the VirtualBox Manager, you can manage VM settings by selecting the VM and clicking on "Settings." Here, you can adjust parameters such as RAM allocation, processors, and storage.

# 11. Snapshot and Clone:

VirtualBox allows you to take snapshots of your VM at different states, providing a backup mechanism. You can also clone VMs for testing or development purposes.

#### 12. Shut Down and Save State:

Properly shut down your VM when finished, either by choosing "Shut Down" from within the guest OS or by selecting the VM in the VirtualBox Manager and clicking the "Close" button. Optionally, you can save the machine state to resume exactly where you left off.

Beware: Saving the machine in state to resume is not very robust, there is a very high chance Virtual Box might crash or not resume from the same point it was paused at, therefore it is advised to save all file and then "shut down" the VM.

# **Additional Resources and Troubleshooting for Virtual Box**

- Virtual Box Documentation: https://www.virtualbox.org/wiki/Documentation
- Virtual Box Manual: <a href="https://www.virtualbox.org/manual/ch01.html">https://www.virtualbox.org/manual/ch01.html</a>
- Virtual Box Forum: <a href="https://forums.virtualbox.org/index.php">https://forums.virtualbox.org/index.php</a> (helpful for finding similar problem queries and solutions)
- Ubuntu Documentation: <a href="https://help.ubuntu.com/">https://help.ubuntu.com/</a>
- Ubuntu Community Support: <a href="https://ubuntu.com/support/community-support">https://ubuntu.com/support/community-support</a>
- Stack overflow: https://stackoverflow.com/ (Public Q&A platform for debugging)



• Bioinformatics (BioStars) Forum: <a href="https://www.biostars.org/t/Forum/">https://www.biostars.org/t/Forum/</a> (General Bioinformatics queries)

# **Introduction to Software Installation**

This subsection provides extensive instructions for software installation on Ubuntu/Windows/MacOS systems, applicable to both virtual machine (VM) and host machine setups, as taught and utilized in the Genomics and Clinical Virology 2024 course. For VM installation specifics, please consult the supplementary VM installation guide attached separately. Additionally, valuable troubleshooting links are provided below for additional assistance.

**Note:** The Virtual Machine file (.vdi) contains all the software installed for the course.

# Software list according to course modules

Module	Software	Summary	Version	Website
Reference	Burrow-	Software package for mapping	0.7.17	https://github.com/lh3/bw
alignment,	Wheeler	short DNA sequences against a		<u>a</u>
coverage and	Aligner	large reference genome, such as		
stats	(BWA)	the human genome.		
Reference	Bowtie2	Tool for aligning sequencing	2.5.2	https://github.com/BenLan
alignment,		reads to long reference		gmead/bowtie2
coverage and		sequences.		
stats				
Reference	samtools	Suite of programs for interacting		https://www.htslib.org/
alignment, coverage and		with high-throughput	1.19	
stats/ Variant		sequencing data.		
calling				
Reference	weeSAM	Provides information on breadth	1.6	https://github.com/centre-
alignment,		and depth coverage of a SAM		for-virus-
coverage and		file.		research/weeSAM/tree/m
stats				<u>aster</u>
Reference	Tablet	Lightweight, high-performance		https://github.com/cropge
alignment,		graphical viewer for next		eks/tablet
coverage and		generation sequence assemblies	1.17.08	
stats		and alignments.	.17	
Reference	iVar	Computational package that		https://github.com/anders
alignment,		contains functions broadly useful		en-lab/ivar
coverage and		for viral amplicon-based		
stats		sequencing.	1.4.2	
Reference	LoFreq	Sensitive variant calling from		
alignment,		sequencing data		https://github.com/CSB5/I
coverage and			245	<u>ofreq</u>
stats			2.1.5	



Reference Qualimap alignment, coverage and	Eventines services discussed		https://github.com/rofiner
	Examines sequencing alignment		https://github.com/refiner y-platform/qualimap2
LCOVERAGE AND L	data in SAM/BAM files and		y-piatiorini/qualimapz
stats	maps reads.	2.3	
Reference Prinseq	Helps pre-processing of genomic	2.3	https://github.com/uwb-
alignment,	and metagenomic sequence data		linux/prinseq
coverage and	in FASTA or FASTQ format.		
stats	III TASTA OF TASTQ TOTTIAL.	0.20.4	
Introduction to SPAdes	Small genome assembler uses de		https://github.com/ablab/s
metagenomics	novo sequencing	3.15.5	<u>pades</u>
Introduction to Centrifuge	Classifier for metagenomic		https://github.com/Daehw
metagenomics	sequences	1.0.4	anKimLab/centrifuge
Introduction to Seqtk	Tool for processing sequences in		https://github.com/lh3/se
metagenomics	the FASTA or FASTQ format	1.4	<u>qtk</u>
Phylogenetic Mafft	Align multiple amino acid or		https://github.com/GSLBio
Analysis	nucleotide sequences.	7.52	tech/mafft
Phylogenetic MEGA-X	Tool for conducting sequence		https://www.megasoftwar
Analysis/	alignment and inferring	11.0.13	e.net/
Phylodynaimcs	phylogenetic trees	-1	
Phylogenetic Modeltest-	Tool for selecting the best-fit		https://github.com/ddarrib
Analysis ng	model of evolution for DNA and		a/modeltest
	protein alignments	0.1.7	
Phylogenetic IQ-TREE	Infer phylogenetic trees by		http://www.iqtree.org/
Analysis	maximum likelihood.	2.2.6	
Phylogenetic Figtree	Graphical viewer of phylogenetic		http://tree.bio.ed.ac.uk/so
Analysis/	trees		ftware/figtree/
Phylodynamics		1.4.4	
Phylogenetic Entrez	Interface into the Entrez query		https://www.ncbi.nlm.nih.
Analysis eutilities	and database	16.2	gov/books/NBK25497/
File Formats & FastQC	Quality control checks on raw		https://www.bioinformatic
QC	sequence data	0.40.4	s.babraham.ac.uk/projects
		0.12.1	/fastqc/
	A wrapper around Cutadapt and		https://github.com/FelixKr
File Formats & Trim Galore			
QC Trim Galore	FastQC to consistently apply		ueger/TrimGalore
	adapter and quality trimming to		
	adapter and quality trimming to FastQ files, with extra	0.0.40	
QC	adapter and quality trimming to FastQ files, with extra functionality for RRBS data	0.6.10	ueger/TrimGalore
	adapter and quality trimming to FastQ files, with extra functionality for RRBS data A conda-smithy repository for		ueger/TrimGalore  https://github.com/conda-
QC Variant calling unzip	adapter and quality trimming to FastQ files, with extra functionality for RRBS data A conda-smithy repository for unzip	6	ueger/TrimGalore  https://github.com/conda-forge/unzip-feedstock
QC	adapter and quality trimming to FastQ files, with extra functionality for RRBS data A conda-smithy repository for unzip De novo assembler designed to		https://github.com/conda- forge/unzip-feedstock https://github.com/sanger-
QC Variant calling unzip	adapter and quality trimming to FastQ files, with extra functionality for RRBS data  A conda-smithy repository for unzip  De novo assembler designed to assemble virus genomes that	6	ueger/TrimGalore  https://github.com/conda-forge/unzip-feedstock
Variant calling unzip  De novo IVA	adapter and quality trimming to FastQ files, with extra functionality for RRBS data  A conda-smithy repository for unzip  De novo assembler designed to assemble virus genomes that have no repeated sequences	6 1.0.11	https://github.com/conda- forge/unzip-feedstock https://github.com/sanger- pathogens/iva
QC Variant calling unzip	adapter and quality trimming to FastQ files, with extra functionality for RRBS data  A conda-smithy repository for unzip  De novo assembler designed to assemble virus genomes that have no repeated sequences  Software which has command	6	https://github.com/conda- forge/unzip-feedstock https://github.com/sanger- pathogens/iva https://github.com/dib-
Variant calling unzip  De novo IVA	adapter and quality trimming to FastQ files, with extra functionality for RRBS data  A conda-smithy repository for unzip  De novo assembler designed to assemble virus genomes that have no repeated sequences  Software which has command line tools for working with DNA	6 1.0.11	https://github.com/conda- forge/unzip-feedstock https://github.com/sanger- pathogens/iva
Variant calling unzip  De novo IVA  De novo khmer	adapter and quality trimming to FastQ files, with extra functionality for RRBS data  A conda-smithy repository for unzip  De novo assembler designed to assemble virus genomes that have no repeated sequences  Software which has command line tools for working with DNA shotgun sequencing data	6 1.0.11 2.1.2	https://github.com/conda- forge/unzip-feedstock https://github.com/sanger- pathogens/iva https://github.com/dib- lab/khmer
Variant calling unzip  De novo IVA	adapter and quality trimming to FastQ files, with extra functionality for RRBS data  A conda-smithy repository for unzip  De novo assembler designed to assemble virus genomes that have no repeated sequences  Software which has command line tools for working with DNA shotgun sequencing data  Quality Assessment tool,	6 1.0.11	https://github.com/conda-forge/unzip-feedstock https://github.com/sanger-pathogens/iva https://github.com/dib-lab/khmer https://github.com/ablab/
Variant calling unzip  De novo IVA  De novo khmer	adapter and quality trimming to FastQ files, with extra functionality for RRBS data  A conda-smithy repository for unzip  De novo assembler designed to assemble virus genomes that have no repeated sequences  Software which has command line tools for working with DNA shotgun sequencing data	6 1.0.11 2.1.2	https://github.com/conda- forge/unzip-feedstock https://github.com/sanger- pathogens/iva https://github.com/dib- lab/khmer



De novo	Spades	Open source genome assembler tool for de novo sequencing		https://github.com/ablab/s pades
De novo	Trimmomat ic	Read trimming tool for illumina NGS Data	0.39	https://github.com/usadellab/Trimmomatic
Phylodynamics	Tempest	Tool for investigating the temporal signal and 'clocklikeness' of molecular phylogenies.	2.0.3	https://github.com/beast- dev/Tempest/blob/main/R EADME.md
Phylodynamics	Tracer	Program for analysing the trace files generated by Bayesian MCMC runs	1.7.2	https://github.com/beast- dev/tracer
Phylodynamics	BEAST (includes BEAGULE, TreeAnnota tor and BEAUti plugin)	High-performance library that can perform the core calculations at the heart of most Bayesian and Maximum Likelihood phylogenetics package.	1.10.4. 0	https://github.com/bioDS/beast-phylonco Also refer for documentation: https://beast.community/first_tutorial
Phylodynamics	Google Earth	Google Earth is a computer program that renders a 3D representation of Earth based primarily on satellite imagery.	7.3.4	https://maps.google.co.uk/ intl/en_uk/earth/

**Note:** The versions might differ as new releases are enrolled by the software company.

# **Installation of Python and Python Installer (Anaconda)**

# For Windows:

- 1. Visit the official Python website (<a href="https://www.python.org/">https://www.python.org/</a>).
- 2. Navigate to the "Downloads" section and download the latest version of Python for Windows.
- 3. Run the Installer:
  - Double-click the downloaded installer (e.g., python-3.x.x.exe).
  - Follow the on-screen instructions, selecting "Add Python to PATH" during installation.
- 4. Verify Installation: Open the Command Prompt and type python --version to confirm the Python version.

# For macOS:

- 1. Install Python using Anaconda: Download the Anaconda distribution from the official website (<a href="https://www.anaconda.com/products/distribution">https://www.anaconda.com/products/distribution</a>).
- 2. Follow the installation instructions for macOS.
- 3. Verify Installation: In Terminal, type python --version to confirm the Python version.

#### For Linux:



- 1. Install Python using Package Manager:
- 2. Run sudo apt-get install python3 for Debian/Ubuntu or sudo yum install python3 for Red Hat/Fedora.
- 3. Verify Installation: Open Terminal and type python3 --version to confirm the Python version.

# **Installing R and RStudio**

### For Windows:

- 1. Download R Installer: Visit the CRAN website (<a href="https://cran.r-project.org/mirrors.html">https://cran.r-project.org/mirrors.html</a>).
- 2. Select a mirror and download the latest version of R for Windows.
- 3. Run the Installer: Double-click the downloaded installer (e.g., R-4.x.x-win.exe).
- 4. Follow the on-screen instructions, selecting default settings.
- 5. Download RStudio from the official website (https://www.rstudio.com/products/rstudio/download/).
- 6. Follow the installation instructions for your operating system.
- 7. Verify Installation: Open RStudio and check the R version using version.

#### For macOS:

- 1. Install Python using Anaconda: Download the Anaconda distribution from the official website (<a href="https://www.anaconda.com/products/distribution">https://www.anaconda.com/products/distribution</a>).
- 2. Follow the installation instructions for macOS.
- 3. Verify Installation: In Terminal, type R --version to confirm the R version.

### For Linux:

- 1. Install R using Package Manager: Run sudo apt-get install r-base for Debian/Ubuntu or sudo yum install R for Red Hat/Fedora.
- 2. Install RStudio: Download RStudio from the official website (<a href="https://www.rstudio.com/products/rstudio/download/">https://www.rstudio.com/products/rstudio/download/</a>).
- 3. Follow the installation instructions for your operating system.
- 4. Verify Installation: Open RStudio and check the R version using version.

# **Software Installation via Shell Scripting**

#### **Conda Overview:**

Conda is an open-source package management and environment management system that runs on Windows, macOS, and Linux. It simplifies the installation and management of software packages, ensuring dependencies are correctly handled.

# **Installation Script:**

Ensure you have Conda installed on your system before running the script.



1. Create a Conda Environment (Optional): If you prefer to create a separate environment for these tools, you can do so by running:

# Create Conda environment conda create -n bioinformatics python

2. Add Conda Channels: Add necessary channels for accessing bioinformatics packages:

# # Add necessary Conda channels conda config --add channels defaults conda config --add channels bioconda conda config --add channels conda-forge

3. Installations of software and verify:

# Create Conda environment conda create -n bioinformatics python

# Activate Conda environment conda activate bioinformatics

# Install and Verify BWA conda install bwa bwa --version

# Install and Verify Bowtie2 conda install bowtie2 bowtie2 --version

# Install and Verify Samtools conda install samtools samtools --version

# Install and Verify weeSAM conda install weesam weesam --version

# Install and Verify Tablet conda install tablet tablet --version

# Install and Verify iVar conda install ivar ivar version



# # Install and Verify LoFreq conda install lofreq lofreq version

# # Install and Verify Qualimap conda install qualimap2 qualimap --version

# # Install and Verify Prinseq conda install prinseq prinseq --version

# # Install and Verify SPAdes conda install spades spades.py --version

# # Install and Verify Centrifuge conda install centrifuge centrifuge --version

# # Install and Verify Seqtk conda install seqtk seqtk

# # Install and Verify Mafft conda install mafft mafft --version

# # Install and Verify MEGA-X conda install mega-x megacc --version

# # Install and Verify Modeltest-ng conda install modeltest-ng modeltest-ng --version

# # Install and Verify IQ-TREE conda install iqtree iqtree --version

# # Install and Verify Figtree conda install figtree figtree --version



# # Install and Verify FastQC

conda install fastqc fastqc --version

# # Install and Verify Trim Galore

conda install trim-galore trim galore --version

# # Install and Verify Unzip

conda install unzip unzip

# # Install and Verify IVA

conda install iva iva --version

### # Install and Verify khmer

conda install khmer interleave-reads.py --version

# # Install and Verify Quast

conda install quast quast.py --version

# # Install and Verify Trimmomatic

conda install trimmomatic trimmomatic --version

# # Install and Verify Tempest

conda install tempest tempest --version

# # Install and Verify Tracer

conda install tracer tracer --version

# # Install and Verify BEAGLE

conda install beagle beagle --version

# # Install and Verify BEAST

conda install beast beast --version



**Note:** In order to install individual software, use the command line command "conda install softwareName". For example: conda install spades.

4. If you created a separate environment, deactivate it:

# Deactivate Conda environment conda deactivate

#### Note:

- Conda environments provide isolation for different sets of tools, enhancing reproducibility.
- You can customize the script based on your preferences, such as creating a dedicated environment or modifying the channels. Activate the Conda base environment (conda activate base) if you choose not to create a separate environment.
- By using Conda, this script streamlines the installation process, ensuring that the specified bioinformatics tools and their dependencies are correctly configured on your system.
- Save this script to a file (e.g., install\_bioinformatics.sh), make it executable (chmod +x install\_bioinformatics.sh), and run it in your terminal (./install\_bioinformatics.sh). Adjust the script as needed for your specific requirements.

# **Installing Google Earth**

# For Windows/Mac:

- 1. Visit the Google Earth download page (<a href="https://maps.google.co.uk/intl/en\_uk/earth/">https://maps.google.co.uk/intl/en\_uk/earth/</a>) in your web browser.
- 2. Click on the "Agree and Download" button to download the installer.
- 3. Once the download is complete, locate the downloaded file (usually in your Downloads folder) and double-click on it to run the installer.
- 4. Follow the on-screen instructions provided by the installer. You may be asked to confirm permissions or choose an installation location.
- 5. After the installation is complete, you should find a Google Earth icon on your desktop or in your Start menu.
- 6. Double-click the Google Earth icon to launch the application.

#### For Linux:

- 1. Google Earth for Linux is available as a .deb or .rpm package. Choose the appropriate package for your Linux distribution.
- 2. Visit the Google Earth download page (<a href="https://maps.google.co.uk/intl/en\_uk/earth/">https://maps.google.co.uk/intl/en\_uk/earth/</a>) in your web browser.



- 3. Download the .deb or .rpm package depending on your distribution.
- 4. Open a terminal and navigate to the directory where the downloaded package is located.
- 5. Install the package using the package manager for your distribution. For example, on Debian-based systems (like Ubuntu), you can use the following command: sudo dpkg -i google-earth-prostable current amd64.deb
- 6. Replace "google-earth-pro-stable\_current\_amd64.deb" with the actual name of the downloaded file
- 7. Once the installation is complete, you can launch Google Earth from the applications menu or by running google-earth-pro in the terminal.

**Note:** Remember to check the official Google Earth website for any updated installation instructions or changes.

# **Additional Resources and Troubleshooting for Software Installations**

- Ubuntu Documentation: https://help.ubuntu.com/
- Ubuntu Community Support: <a href="https://ubuntu.com/support/community-support">https://ubuntu.com/support/community-support</a>
- Conda Installation: https://conda.io/projects/conda/en/latest/user-guide/install/index.html
- Conda Documentation: <a href="https://conda.io/projects/conda/en/latest/user-guide/getting-started.html#managing-python">https://conda.io/projects/conda/en/latest/user-guide/getting-started.html#managing-python</a>
- Stack overflow: <a href="https://stackoverflow.com/">https://stackoverflow.com/</a> (Public Q&A platform for debugging)
- Bioinformatics (BioStars) Forum: <a href="https://www.biostars.org/t/Forum/">https://www.biostars.org/t/Forum/</a> (General Bioinformatics queries)