

MEDICAL MICROBIOLOGY AND INFECTIOUS DISEASES BIOINFORMATICS WORKSHOP

Presents

Introduction to conda and Tool installation

INSTRUCTED BY

Grace E. Seo, MSc Student



INFORMATION FOR PARTICIPANTS

All workshops are being recorded and posted to the MMID Bioinformatics Workshop - YouTube

For live Q&A, go to <u>slido.com</u> and use participant code #9406658

2023 MMID Bioinformatics Workshop Schedule

DATE	INSTRUCTOR	TOPIC
March 2	Grace E. Seo	Introduction to the 2023 MMID Bioinformatics Workshop
March 9	Grace E. Seo	Introduction to conda and tool installation
March 16	Grace E. Seo	Introduction to genomics and viral data analysis
March 23	Jill Rumore	Bacterial Genomics
March 30	Jill Rumore	Reference Databases
April 6	Taylor Davedow	Beginner's Guide to Phylogenetic Trees
April 13	Taylor Davedow	Introduction to tree visualization and annotation using ggtree
April 20	-	Bfx workshop: Bring your own dataset!
April 27	-	Bfx workshop: Bring your own dataset!

April 20 and April 27 in-person sessions are open to the public (up to 100 people)!

Work with your colleagues/friends to analyze data together.

SET UP WI-FI (IN-PERSON PARTICIPANTS)

- 1. Connect to UofM-secure (if you are a student or staff)
 - Use your @myumanitoba.ca or @umanitoba.ca login and password

2. Connect to UofM-guest

To access uofm-guest Wi-Fi:

- Ensure your wireless card is active and connected to the uofm-guest network.
- Open your web browser (e.g. Google Chrome, Microsoft Edge, Firefox, etc.) and browse to any website. This should redirect you to the Acceptable Use Agreement page.
- 3. Review the Acceptable Use Agreement for the unsecured wireless.
- 4. Select I Agree.

- 1. Describe method to install Ubuntu using PowerShell (Windows user)
- 2. Describe the purpose of GitHub and provide usage overview.
- 3. Provide basic overview of BASH commands.
- 4. Practice navigating through the terminal using commands.
- 5. <u>Describe terminal permission structure for files.</u>
- 6. Describe the purpose of conda.
- 7. Install conda environment and tools.

- 1. Describe method to install Ubuntu using PowerShell (Windows user)
- 2. Describe the purpose of GitHub and provide usage overview.
- 3. Provide basic overview of BASH commands.
- 4. Practice navigating through the terminal using commands.
- 5. Describe terminal permission structure for files.
- 6. Describe the purpose of conda.
- 7. Install conda environment and tools.

Windows WSL PowerShell

If you have enabled WSL but cannot find Ubuntu on Microsoft Store,

seog@SMARTY: ~

use command line to install.

- 1. Open PowerShell as administrator
- 2. Type the following command
- >wsl --install -d ubuntu

```
Welcome to Ubuntu 22.04.1 LTS (GNU/Linux 5.10.16.3-microsoft-standard-WSL2 x86_64)
* Documentation: https://help.ubuntu.com
* Management: https://landscape.canonical.com
* Support: https://ubuntu.com/advantage

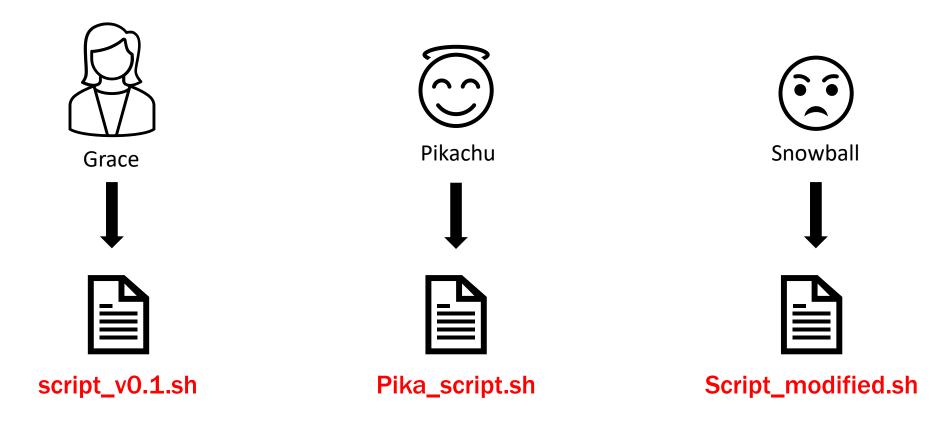
This message is shown once a day. To disable it please create the /home/seog/.hushlogin file.
seog@SMARTY:~$
```

```
Administrator: Windows PowerShell
Windows PowerShell
Copyright (C) Microsoft Corporation. All rights reserved.

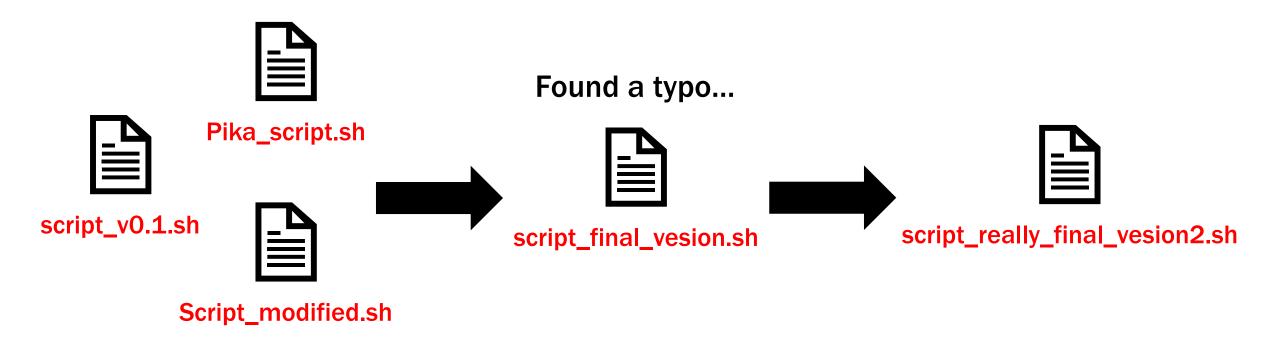
Install the latest PowerShell for new features and improvements! https://aka.ms/PSWindows
PS C:\WINDOWS\system32> wsl --install -d ubuntu_
```

- 1. Describe method to install Ubuntu using PowerShell (Windows user)
- 2. Describe the purpose of GitHub and provide usage overview.
- 3. Provide basic overview of BASH commands.
- 4. Practice navigating through the terminal using commands.
- 5. Describe terminal permission structure for files.
- 6. Describe the purpose of conda.
- 7. Install conda environment and tools.

Project: build analysis pipeline



How to merge all versions into one final script...



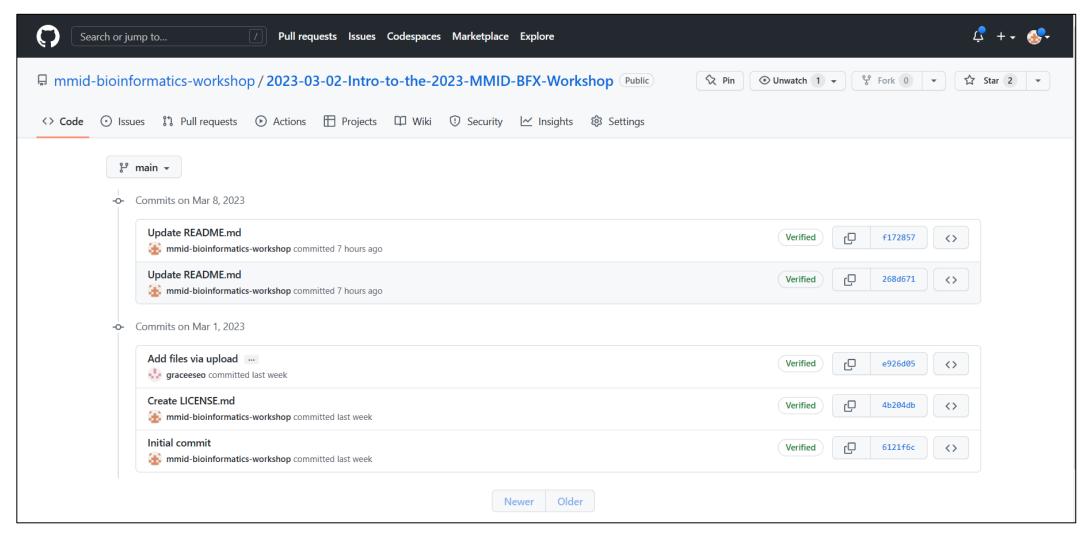
- 1. Git is an open-source version control system software that tracks changes.
- 2. Changes are tracked for easy comparison.
- 3. You can find out what was changed in each update.





https://code.visualstudio.com/docs/sourcecontrol/overview

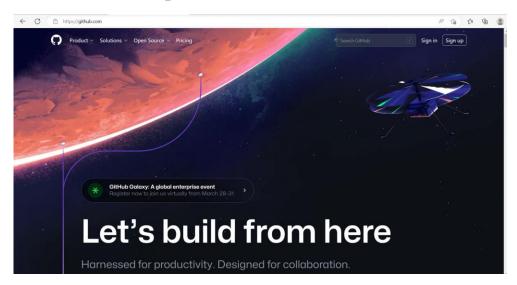
- 1. Git is an open-source version control system software that tracks changes.
- 2. Changes are tracked for easy comparison.
- 3. You can find out what was changed in each update.







- GitHub is a Git repository hosting service with webbased graphical interface.
- We will use GitHub to share workshop related contents, data, scripts and PowerPoint slides.



GitHub usage

Demonstration

- 1. Describe method to install Ubuntu using PowerShell (Windows user)
- 2. Describe the purpose of GitHub and provide usage overview.
- 3. Provide basic overview of BASH commands.
- 4. Practice navigating through the terminal using commands.
- 5. Describe terminal permission structure for files.
- 6. Describe the purpose of conda.
- 7. Install conda environment and tools.



Current directory

USERNAME@COMPUTER_NAME:/Desktop\$

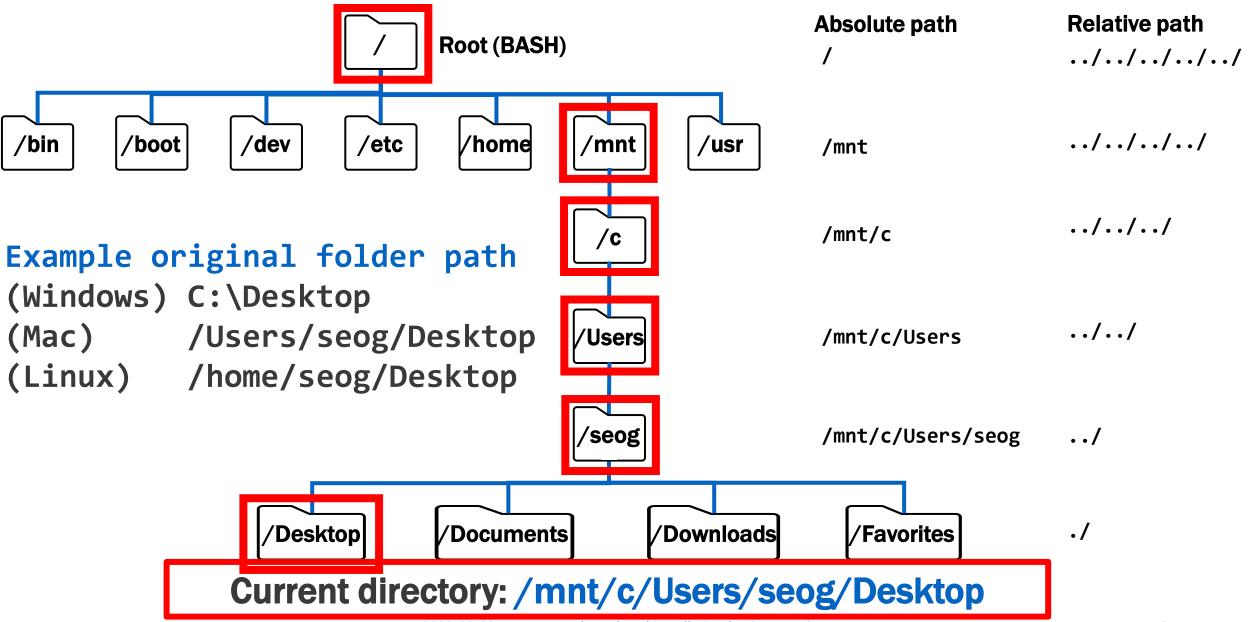
seog@Smarty:.../Desktop\$

Prompt - Input command

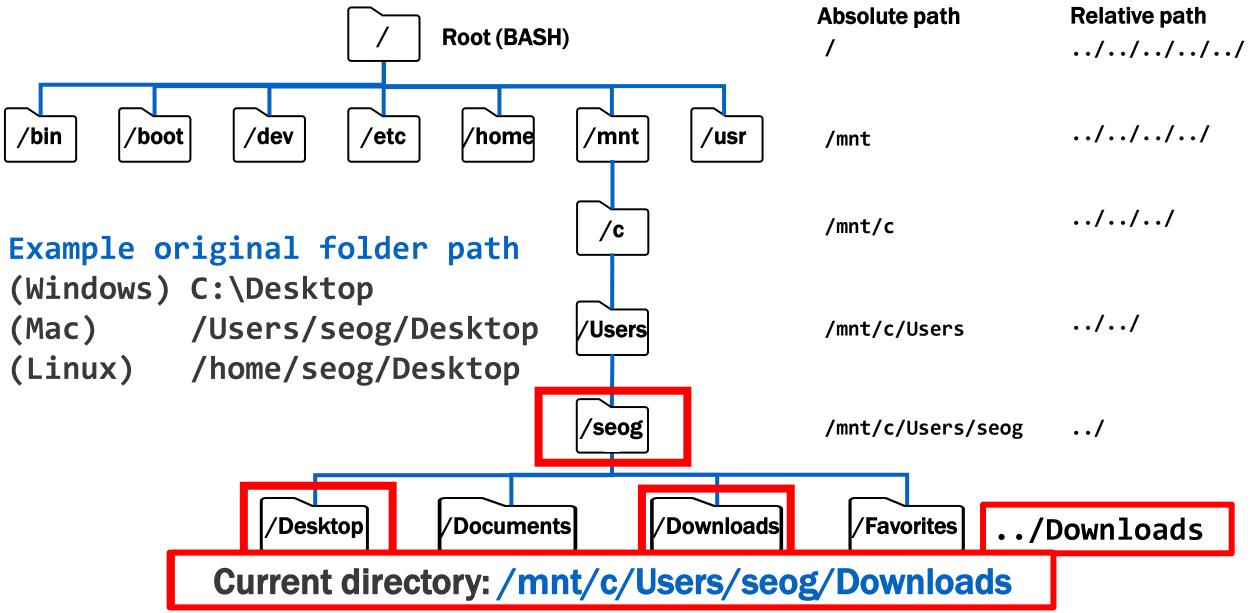
If there is no prompt, either job is in progress or wrong command stalled your terminal

To get your prompt back
(Windows / Linux) Press ctrl-c
(Mac) Press command-c

Example Windows Subsystem for Linux BASH folder structure



Example Windows Subsystem for Linux BASH folder structure



BASH commands

- Print working directory
- List directory content
- Change directory
- Create directory
- Create a file
- Rename file/directory
- Move file/directory
- Copy file/directory

- \$ pwd
- \$ 1s \$ 11
- \$ cd
- \$ mkdir
- \$ touch
- \$ mv OLDNAME NEWNAME
- \$ mv FILE NEWPLACE
- \$ cp FILE NEWCOPY

- 1. Describe method to install Ubuntu using PowerShell (Windows user)
- 2. Describe the purpose of GitHub and provide usage overview.
- 3. Provide basic overview of BASH commands.
- 4. Practice navigating through the terminal using commands.
- 5. Describe terminal permission structure for files.
- 6. Describe the purpose of conda.
- 7. Install conda environment and tools.

BASH Basics

Demonstration

- 1. Describe method to install Ubuntu using PowerShell (Windows user)
- 2. Describe the purpose of GitHub and provide usage overview.
- 3. Provide basic overview of BASH commands.
- 4. Practice navigating through the terminal using commands.
- 5. Describe terminal permission structure for files.
- 6. Describe the purpose of conda.
- 7. Install conda environment and tools.

File information and permission

r: readable

w: writable

x: executable

```
Permission ($ chmod ###)
```

```
No permission --- --- rwx rwx
```

Bit: 421 421 421

Triad: Owner group others

```
$ chmod 755 test0001.txt
Owner(rwx) group(r-x) others(r-x)
```

```
$ chmod a+wxr test0001.txt
Owner(rwx) group(rwx) others(rwx)
```

File information and permission

Demonstration

- 1. Describe method to install Ubuntu using PowerShell (Windows user)
- 2. Describe the purpose of GitHub and provide usage overview.
- 3. Provide basic overview of BASH commands.
- 4. Practice navigating through the terminal using commands.
- 5. Describe terminal permission structure for files.
- 6. Describe the purpose of conda.
- 7. Install conda environment and tools.

Conda guide (2022)

Jill Rumore's Conda lecture (2022):

https://github.com/MMID-codingworkshop/2022-01-19-Introduction-to-CONDA

MMID Coding Workshop YouTube (2022-01-19):

https://www.youtube.com/watch?v=r-wmmhjHFJ4



What is conda?

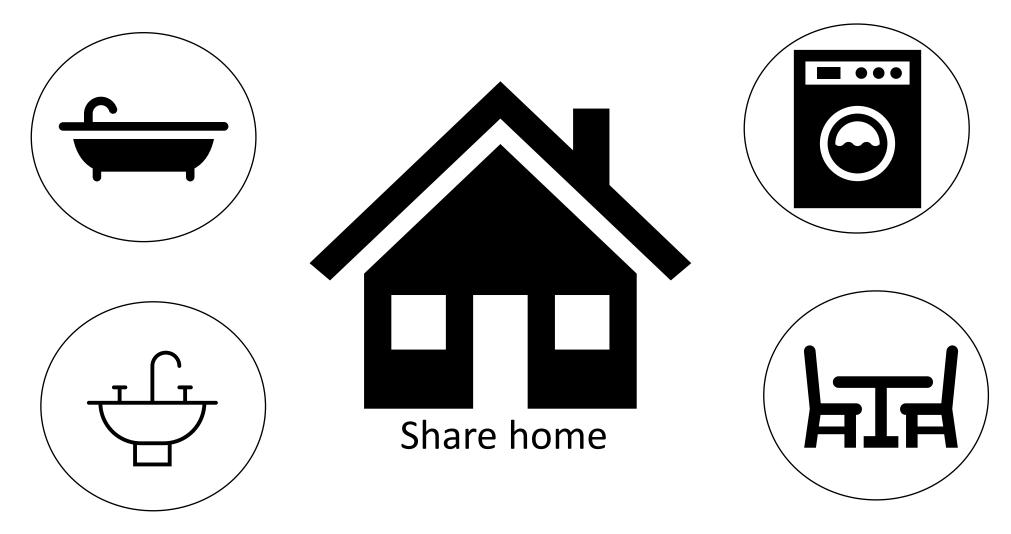
 conda-forge: Most dependencies (numpy, scipy, zlib, CRAN packages, etc.)

- bioconda: Most bioinformatics packages are available in this channel i.e. (STAR, samtools, DESeq2, etc.)
- defaults: Packages built by Anaconda Inc.

CONDA MINI CONDA ANACONDA = conda + python + base packages = miniconda + 150 high quality packages

https://bioconda.github.io/tutorials/gcb2020.html

What is conda?



Activate (into the room) & deactivate (leave the room) conda environment











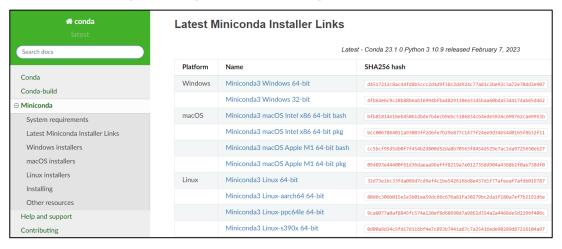
- 1. Describe method to install Ubuntu using PowerShell (Windows user)
- 2. Describe the purpose of GitHub and provide usage overview.
- 3. Provide basic overview of BASH commands.
- 4. Practice navigating through the terminal using commands.
- 5. Describe terminal permission structure for files.
- 6. Describe the purpose of conda.
- 7. Install conda environment and tools.

1. Update your terminal with dependencies

- \$ sudo apt update
- \$ sudo apt upgrade

2. Click Miniconda3 Linux 64-bit to download .sh script

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



3. Open Terminal (Ubuntu/Terminal)

```
$ cd /Downloads
```

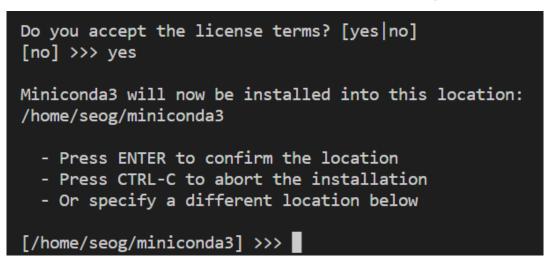
OR \$ cd /mnt/c/Users/USERNAME/Downloads

4. Install Miniconda using bash script

\$ bash Miniconda3-latest-Linux-x86_64.sh

```
seog@SMARTY:/mnt/c/Users/gsezz/Downloads$ bash Miniconda3-latest-Linux-x86_64.sh
Welcome to Miniconda3 py310_23.1.0-1
In order to continue the installation process, please review the license agreement.
Please, press ENTER to continue
>>>
```

- 5. Press q to exit from agreement documentation.
- 6. Type "yes" and press ENTER to accept the license terms.
- 7. Press ENTER to install the software (~1-2 mins)



8. Type "yes" to initialization and press ENTER

9. Close and re-open the terminal for the changes to take

effect.

```
Do you wish the installer to initialize Miniconda3
by running conda init? [yes no]
[no] >>> yes
no change
              /home/seog/miniconda3/condabin/conda
              /home/seog/miniconda3/bin/conda
no change
              /home/seog/miniconda3/bin/conda-env
no change
no change
              /home/seog/miniconda3/bin/activate
              /home/seog/miniconda3/bin/deactivate
no change
no change
              /home/seog/miniconda3/etc/profile.d/conda.sh
              /home/seog/miniconda3/etc/fish/conf.d/conda.fish
              /home/seog/miniconda3/shell/condabin/Conda.psm1
no change
              /home/seog/miniconda3/shell/condabin/conda-hook.ps1
no change
              /home/seog/miniconda3/lib/python3.10/site-packages/xontrib/conda.xsh
no change
              /home/seog/miniconda3/etc/profile.d/conda.csh
no change
modified
              /home/seog/.bashrc
==> For changes to take effect, close and re-open your current shell. <==
If you'd prefer that conda's base environment not be activated on startup,
   set the auto activate base parameter to false:
conda config --set auto_activate_base false
Thank you for installing Miniconda3!
seog@SMARTY:/mnt/c/Users/gsezz/Downloads$
```

Install conda environment

10. Verify installation by checking conda version.

\$ conda --version

```
(base) seog@SMARTY:/mnt/c/Users/gsezz$ conda --version
conda 23.1.0
```

Navigating through conda

- Conda help manual
- Conda command help page
- List of installed environments
- Search for conda packages

- \$ conda --help
- \$ conda COMMAND --help
- \$ conda env list
- \$ conda search PACKAGENAME

- Core commands: create, list, search, install, update, remove

```
(base) seog@SMARTY:/mnt/c/Users/gsezz$ conda env list
# conda environments:
#
base * /home/seog/miniconda3
```

Install conda environment

1. Install conda environment named conda_workshop

```
$ conda create --yes --name conda_workshop
```

(base) seog@SMARTY:/mnt/c/Users/gsezz\$ conda create -y -n conda_workshop

```
Preparing transaction: done
Verifying transaction: done
Executing transaction: done

#

# To activate this environment, use

#

# $ conda activate conda_workshop

#

# To deactivate an active environment, use

#

# $ conda deactivate

(base) seog@SMARTY:/mnt/c/Users/gsezz$
```

Install conda environment

2. Activate conda_workshop environment

\$ conda activate conda_workshop

Install conda package - fastqc

3. Look for the tool availability on Anaconda

ANACONDA. ORG Gallery About Anaconda Help Download Anaconda Search Anaconda.org (Google search) bioconda / packages / fastgc 0.12.1 A quality control tool for high throughput sequence data Google Conda Files Labels Badges fastqc conda License: GPL >=3 ★ Home: http://www.bioinformatics.babraham.ac.uk/projects/fastgc/ Images News + How to use Videos **▲** 618718 total downloads Last upload: 4 days and 16 hours ago About 24.000 results (0.28 seconds) Installers :: Anaconda.org https://anaconda.org > bioconda > fastqc : Info: This package contains files in non-standard labels. Fastgc - :: Anaconda.org A quality control tool for high throughput sequence data. Conda · Files ∆ linux-64 v0.11.8 License: GPL >=3 ... **osx-64** v0.11.8 **ਫ =** ∆ noarch v0.12.1 conda install 🚱 To install this package run one of the following: conda install -c bioconda fastac conda install -c "bioconda/label/broken" fastqc conda install -c "bioconda/label/cf201901" fastqc

Install conda package - fastqc

4. Install conda packages in an environment

```
$ conda list
```

\$ conda install --yes --channel CHANNEL PACKAGENAME

conda install ?

To install this package run one of the following:

```
conda install -c bioconda fastqc
```

```
(conda_workshop) seog@SMARTY:/mnt/c/Users/gsezz$ conda install -y -c bioconda fastqc
Collecting package metadata (current_repodata.json): done
Solving environment: done

## Package Plan ##
environment location: /home/seog/miniconda3/envs/conda_workshop
```

Install conda package - fastqc

5. Check the conda list to verify installation

\$ conda list

```
(conda workshop) seog@SMARTY:/mnt/c/Users/gsezz$ conda list
# packages in environment at /home/seog/miniconda3/envs/conda_workshop:
                          Version
                                                            Channel
# Name
                                                     Build
 libgcc mutex
                                                      main
                          0.1
 openmp mutex
                          5.1
                                                     1 gnu
dbus
                          1.13.18
                                                hb2f20db 0
                                                h6a678d5 0
                          2.4.9
expat
                                                hdfd78af 0
                                                              bioconda
fastqc
                          0.12.1
font-ttf-dejavu-sans-mono 2.37
                                                hd3eb1b0 0
fontconfig
                                                h52c9d5c 1
                          2.14.1
freetype
                                                h4a9f257 0
                          2.12.1
gdbm
                                                hd4cb3f1 4
                           1.18
```

Using the package - fastqc

6. Use the tool command to use (while inside conda environment)

\$ fastqc --help

Updating the package - fastqc

7. Regularly check for tool updates and update package regularly.

\$ conda update --yes PACKAGENAME

```
(conda_workshop) seog@SMARTY:/mnt/c/Users/gsezz$ conda update --yes fastqc
Collecting package metadata (current_repodata.json): done
Solving environment: done

# All requested packages already installed.
```

Deactivate conda environment

8. Leave conda_workshop environment.

\$ conda deactivate

```
(conda_workshop) seog@SMARTY:/mnt/c/Users/gsezz$ conda deactivate
(base) seog@SMARTY:/mnt/c/Users/gsezz$
```

Practice conda package installation

Install the following tools in your conda_workshop environment before the next workshop!

- 1. fastqc (completed)
- 2. minimap2
- 3. vcftools
- 4. samtools
- 5. fastp
- 6. checkM
- 7. Kraken2

LEARNING OBJECTIVES

- 1. Describe method to install Ubuntu using PowerShell (Windows user)
- 2. Describe the purpose of GitHub and provide usage overview.
- 3. Provide basic overview of BASH commands.
- 4. Practice navigating through the terminal using commands.
- 5. Describe terminal permission structure for files.
- 6. Describe the purpose of conda.
- 7. Install conda environment and tools.

HELPFUL RESOURCES - BASH

- 1. What is CLI https://www.hostinger.com/tutorials/what-is-cli
- 2. BASH manual: https://www.gnu.org/software/bash/manual/bash.html
- 3. Information on Linux folder structure https://www.howtogeek.com/117435/htg-explains-the-linux-directory-structure-explained/
- 4. *The BASH Guide: https://guide.bash.academy/
- 5. *Learn Enough Command-Line to be dangerous (free first few chapters): https://www.learnenough.com/command-line-tutorial

YouTube Videos

- 1. *Joe Collins Beginner's Guide to the Bash Terminal: https://www.youtube.com/watch?v=oxuRxtr02Ag
- 2. *Traversy Media Shell Scripting Crash Course Beginner Level:

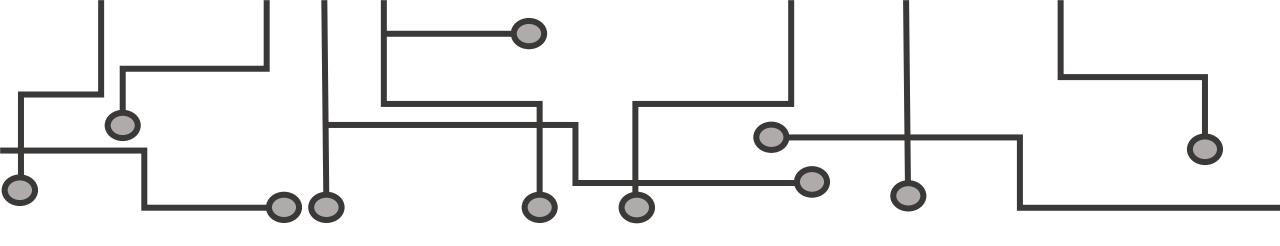
 https://www.youtube.com/watch?v=v-F3YLd6oMw

 2023-03-09 Intro to conda and tool installation by Grace E. Seo

HELPFUL RESOURCES - Conda

- 1. *Jill Rumore's conda workshop (2022-01-19) https://www.youtube.com/watch?v=r-wmmhjHFJ4
- 2. *Jill Rumore's conda workshop GitHub (2022-01-19) https://github.com/MMID-coding-workshop/2022-01-19-Introduction-to-CONDA

- 3. Conda userguide https://docs.conda.io/projects/conda/en/latest/user-guide/getting-started.html
- 4. Conda cheatsheet https://docs.conda.io/projects/conda/en/latest/user-guide/cheatsheet.html
- 5. Conda cheatsheet pdf
 https://docs.conda.io/projects/conda/en/4.6.0/_downloads/52a95608c4967
 1267e40c689e0bc00ca/conda-cheatsheet.pdf



THANK YOU FOR ATTENDING!

Please make sure to fill out the Exit Survey at Slido.com with #9406658

We value your feedback!

More questions? Please email us at mmid.bioinformatics.workshop@gmail.com or post them to the workshop slack channel



Exit survey

Slido Slido.com with #9406658