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SFI Centre for Research Training in GENOMICS DATA SCIENCE

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Introduction to Linux

Speaker: **Declan Bennett**

BennettD@universityofgalway.ie

Who am I

- 2016 - BSc Biotechnology -> psychiatric genetics project
- 2017 - MSc Biomedical Genomics, Genetic variation in the somatic mutation rate
- 2017-2018 – Bioinformatician EMBL-EBI – Accelerating medicines project
- 2018- PhD bioinformatics. Inference of somatic mutation in 200,000 UK biobank exomes.

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Preliminary advice

•Data analysis can be very frustrating, you will make mistakes, and get error messages:

•Expect to spend a large part of your time on Google / forums or learning to use new tools / techniques...

•Don’t run things blindly, always make sure you know how tools / packages work, the stats / biases behind them...

•Data analysis can be as experimental as wet-lab science!

•Tools and applications are constantly evolving, best practices are extremely hard to come by. Computation however doesn’t consume samples / reagents, so don’t be afraid to try new things...

History of UNIX

What is Linux/Unix

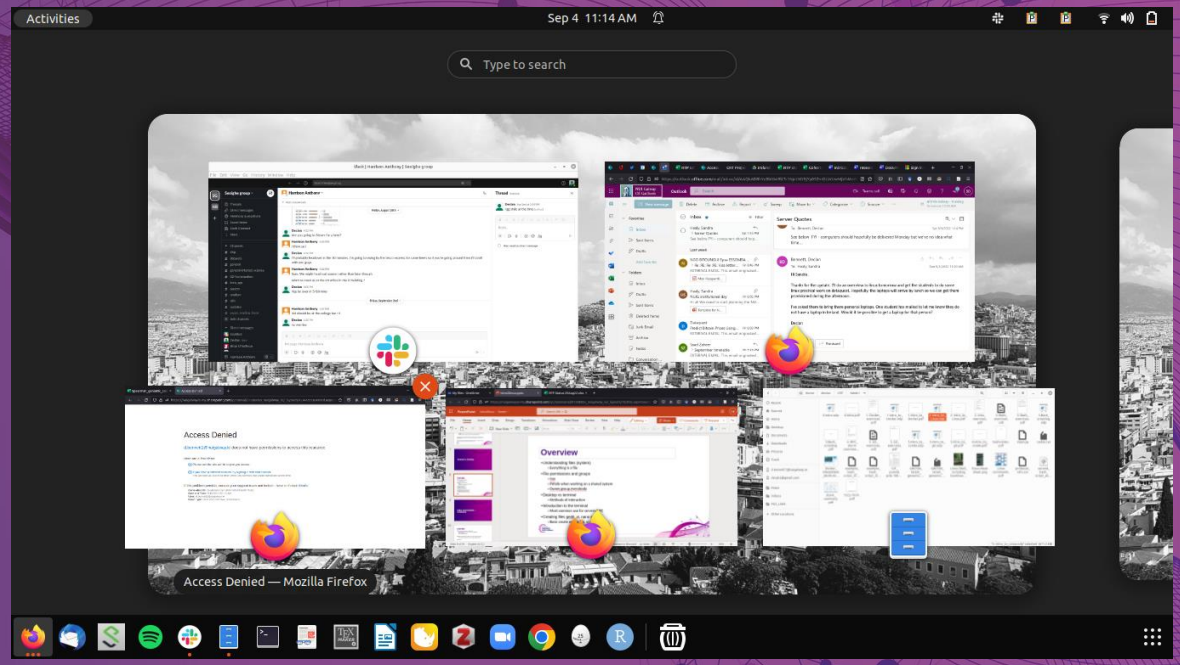
Unix (originally developed at Bell labs in 1960s/70s) is a family of operating systems with some powerful features:

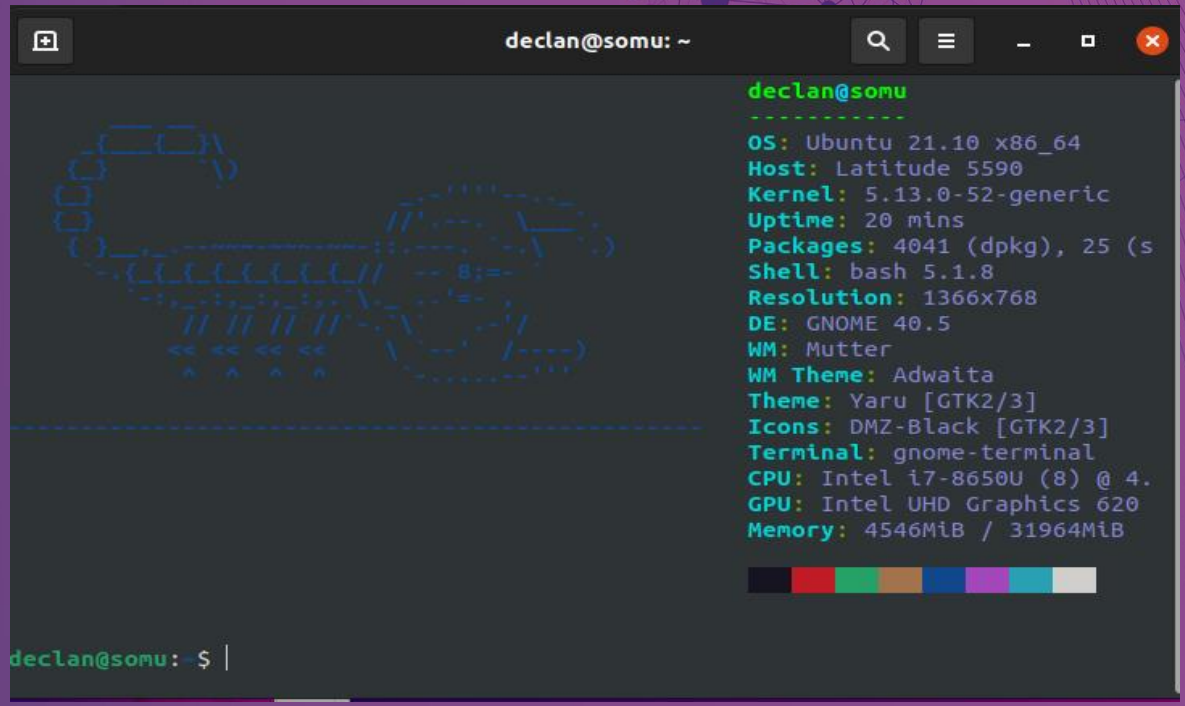
- Stable / Secure - Generally less prone to crashes / hacks
- Efficient multitasking - Designed for a multiuser environment
- Minimalist, modular code ("Do one thing and do it well") written mostly in C – portable
- Unix shell – command line interpreter/interface (CLI), user enters text in a window to execute commands
- Unified File System – "everything is a file" (documents/directories/devices/)

Linux is an open-source Unix-like OS which comes in various distributions - RedHat, Fedora, Debian, etc., etc. Modern variants typically use X11 Windows System plus a desktop environment to provide a GUI.

Most compute clusters (supercomputers) run headless Unix / Linux OS – we usually need to use these types of systems to handle large-scale genomics analyses.

Terminal vs Desktop





Overview

- Understanding files (system)
  - Everything is a file
- File permissions and groups
  - rwx
  - Pitfalls when working on a shared system
  - Owner,group,everybody
- Desktop vs terminal
  - Methods of interaction
- Introduction to the terminal
  - Most common use for servers/HPC
- Creating files gedit, vi, nano etc..
  - Basic create empty file, vi shortcuts

Files

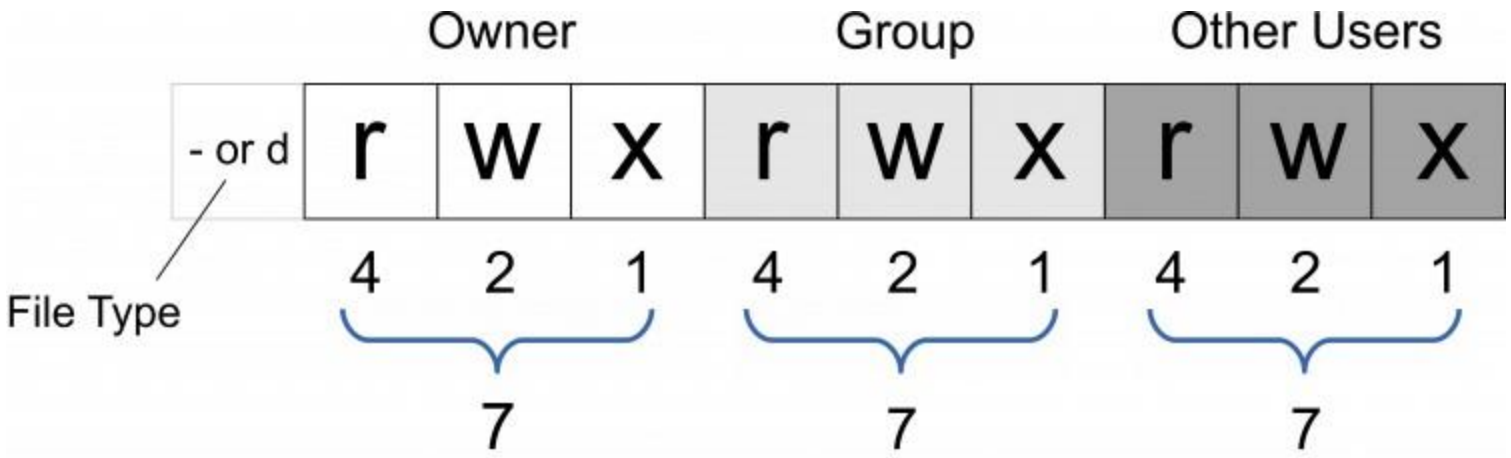
```
declan@somu:~/work/thesis/chapter2$ tree -d -L 1 /
/
├── bin -> usr/bin
├── boot
├── cdrom
├── dev
├── etc
├── home
├── lib -> usr/lib
├── lib32
├── lib64 -> usr/lib64
├── libx32 -> usr/libx32
├── lost+found
├── media
├── mnt
├── opt
├── proc
├── root
├── run
├── sbin -> usr/sbin
├── snap
├── srv
├── sys
├── tmp
├── usr
└── var
```

```
declan@somu:~/work/thesis/chapter2$ l
total 643M
-rw-rw-r-- 1 declan declan 4.1K May 24 10:44 Age_correlations.R
-rw-rw-r-- 1 declan declan  884 May 23 18:25 asymmetry_probes.R
drwxrwxr-x 2 declan declan 4.0K May 25 16:08 batch_corr
-rw-rw-r-- 1 declan declan  665 Jan 14  2022 Check_chr5_assoc.R
drwxrwxr-x 2 declan declan 4.0K May 25 13:00 data
drwxrwxr-x 3 declan declan 4.0K May 24 12:34 expression
drwxrwxr-x 5 declan declan 4.0K Feb 27  2022 gwas
-rw-rw-r-- 1 declan declan 643M Jan 14  2022 old_counts.norm
drwxrwxr-x 2 declan declan 4.0K May 19 11:42 pheno_norm
drwxrwxr-x 2 declan declan 4.0K Apr  5 11:48 pipeline
-rw-rw-r-- 1 declan declan 8.8K May 25 09:39 probe_asymmetry_df.txt
```

Multiple user system

```
dbennett@lugh:/data/Seoighe_data$ ls -l
total 984
drwxrwxr-x 3 dbennett seoighe_group     45 Nov 15  2019 1KG
drwxrwxr-x 4 dbennett dbennett          42 Dec 10  2019 Apples
drwxrwxr-x 4 dbennett seoighe_group   8192 Apr 19 11:00 GTEx
drwxr-x--- 7 scleary  seoighe_group    111 Feb 24  2022 ICGC
drwxrwxr-x 2 scleary  seoighe_group    167 May 14  2020 mapability
drwxrwxr-x 2 scleary  scleary           10 Nov 20  2019 Pennychuik
```

File permissions



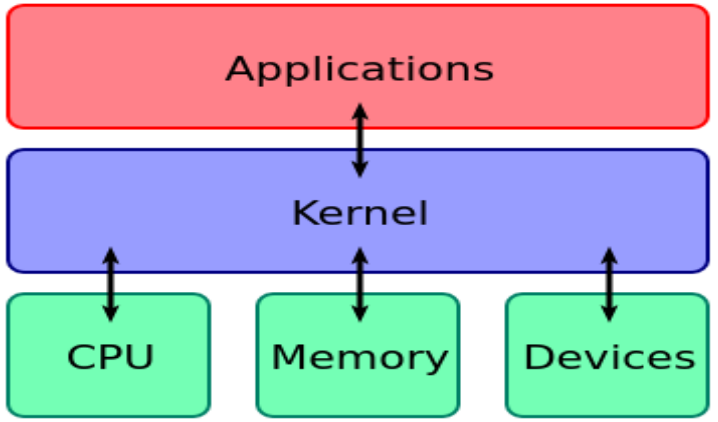
Paths, environments + commands

Overview

- Paths, environment, bashrc + profile, alias’
  - How does the computer know where an executable file is
  - How to specify
  - Some example bash alias’
- Example commands cd, ls, mkdir, rm, top, less, cat, grep, zcat, pipe
  - Moving about, making files, directories, zipping, peaking at files etc...
- Exercises

Processes

Overview



- All instructions from outside of the kernel space are executed in the context of processes
- A process can be seen as a set of instructions with controlled data attached to it
- The top command can be used to list these processes
- The processes information is stored under /proc/PID/

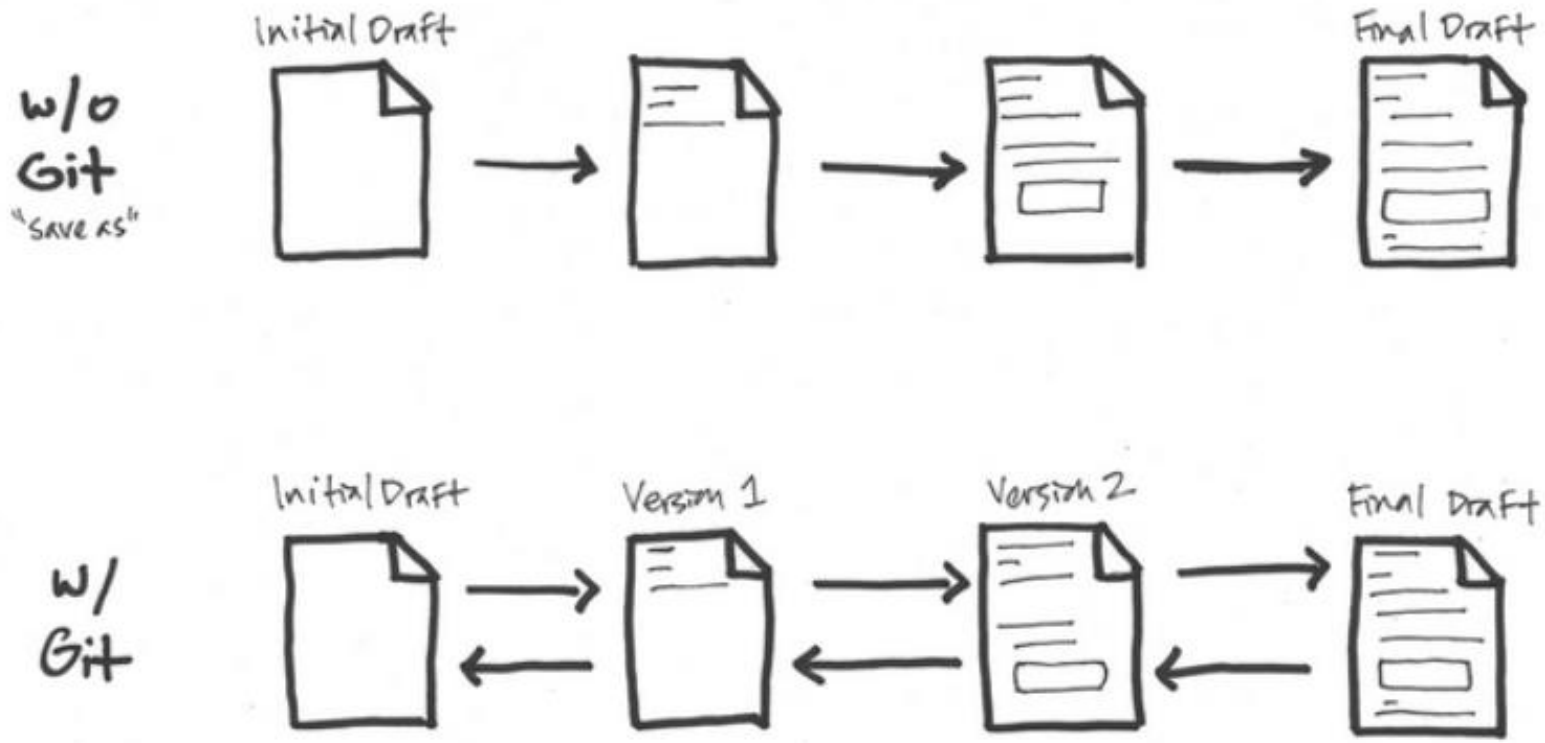
Git


"FINAL".doc
FINAL.doc!
FINAL_rev.2.doc
FINAL_rev.6.COMMENTS.doc
FINAL_rev.8.comments5.
CORRECTIONS.doc
track changes
FINAL_rev.18.comments7.
corrections9.MORE.30.doc
FINAL_rev.22.comments49.
corrections.10.#@$%WHYDID
ICOMETOGRADSCHOOL????.doc
JORGE CHAM © 2012
WWW.PHDCOMICS.COM

- Methodology in software development that ensures all changes to a software project (and code) are tracked in time.

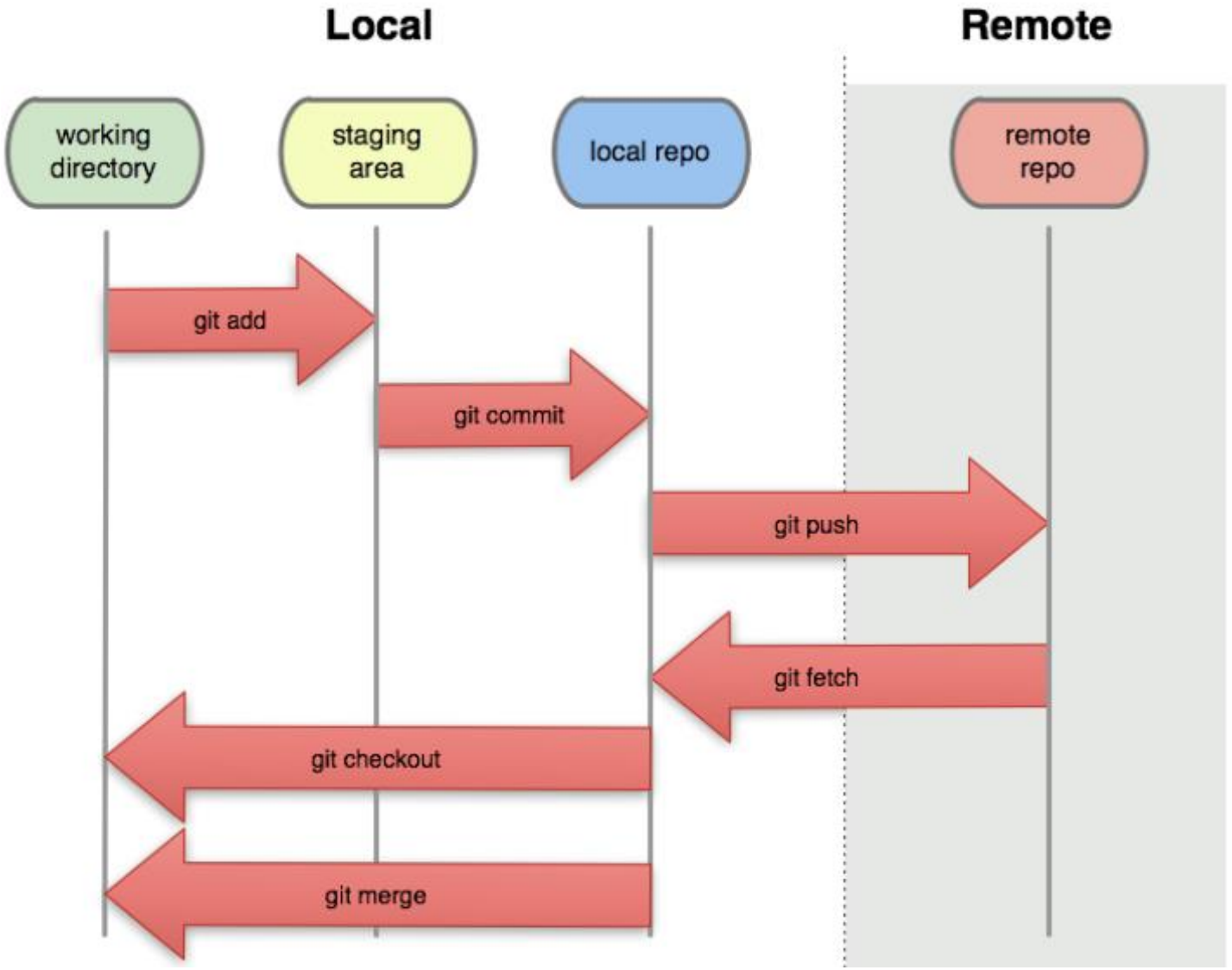
- Advantages
  - you can revert back to specific ‘versions’ of your code
  - collaboration becomes practical, as specific changes and associated contributors are tracked

- The most commonly used version control systems is Git

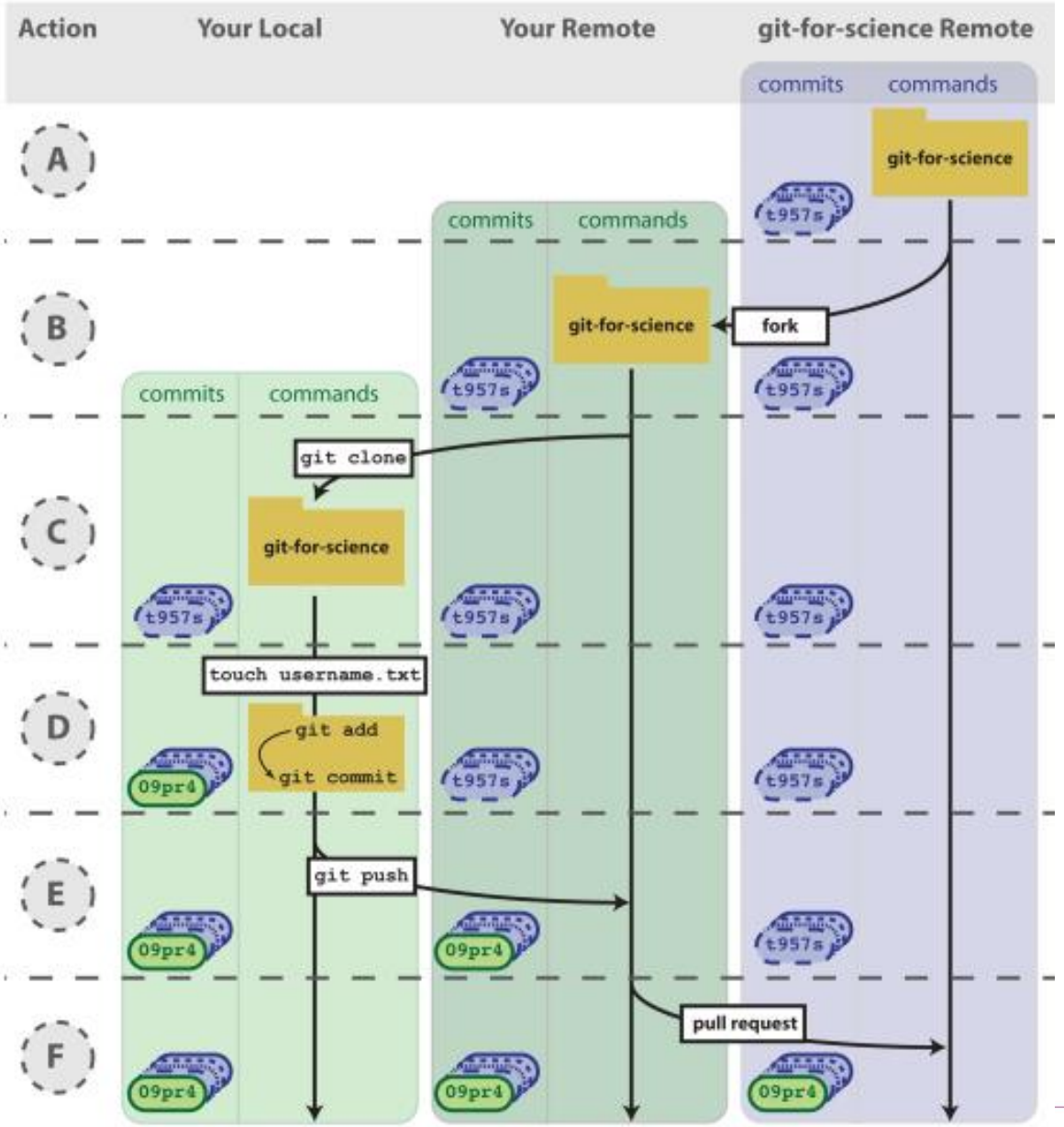


'Edits' etc. are easily forgotten - with *git* all changes are logged

Version Control with Git



Collaborative software



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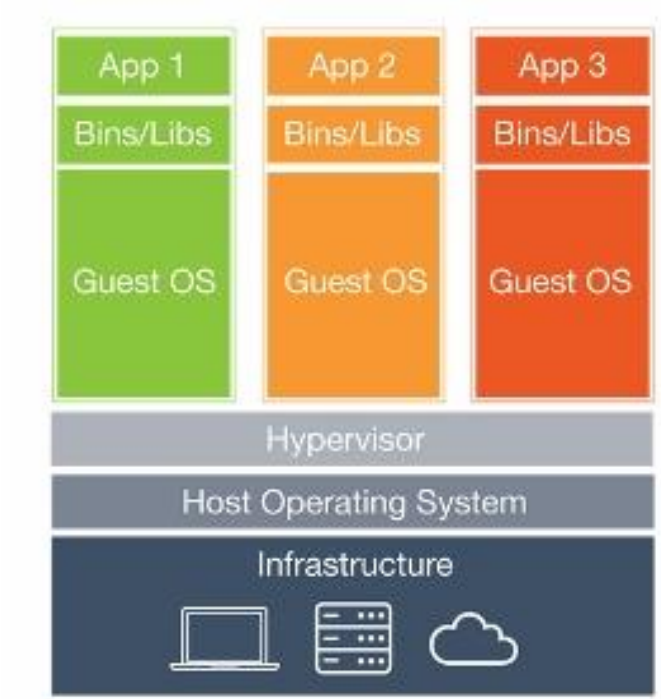
Github readme

Introduction to bash scripting

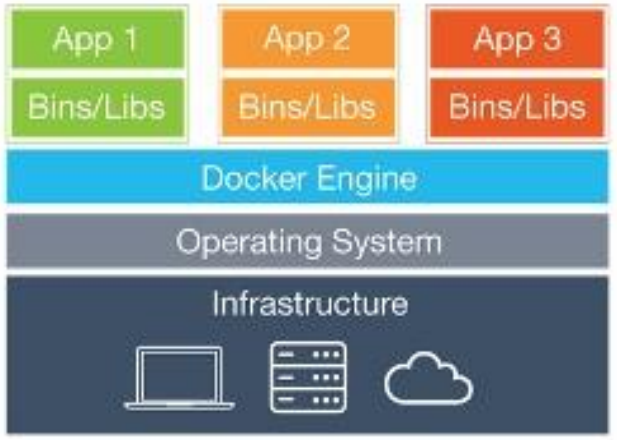
Containers

Overview

•Difference between virtual machines and containers



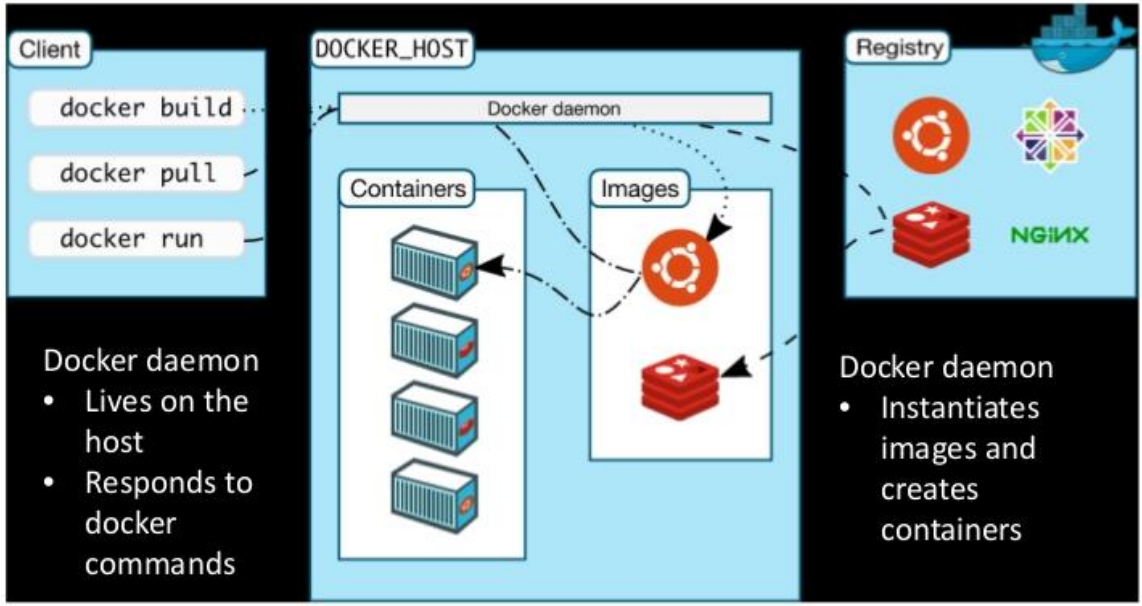
Virtual Machines



Containers

Core concepts

- Docker Image: read-only template with instructions for creating a container
- Docker Container: a runnable instance of an image
- Docker Registry: ‘App-store’ for Docker images. Docker is configured to use Docker Hub by default.
- Dockerfile: set of instructions to build an image



Core commands and options

command	description
`docker images`	list all local images
`docker history` *image*	show the image history (list of ancestors)
`docker inspect` *image...*	show low-level infos (in json format)
`docker tag` *image tag*	tag an image
`docker commit` *container image*	create an image (from a container)
`docker import` *url*|- [*tag*]	create an image (from a tarball)
`docker rmi` *image...*	delete images

command	description
`docker create` *image* [*command*]	create the container
`docker run` *image* [*command*]	= `create` + `start`
`docker rename` *container new_name*	rename the container
`docker update` *container*	update the container config
`docker start` *container...*	start the container
`docker stop` *container...*	graceful[2] stop
`docker kill` *container...*	kill (SIGKILL) the container
`docker restart` *container...*	= `stop` + `start`
`docker pause` *container...*	suspend the container
`docker unpause` *container...*	resume the container
`docker rm` [`-f`[3]] *container...*	destroy the container

[2] send SIGTERM to the main process + SIGKILL 10 seconds later

[3] `-f` allows removing running containers (= `docker kill` + `docker rm`)

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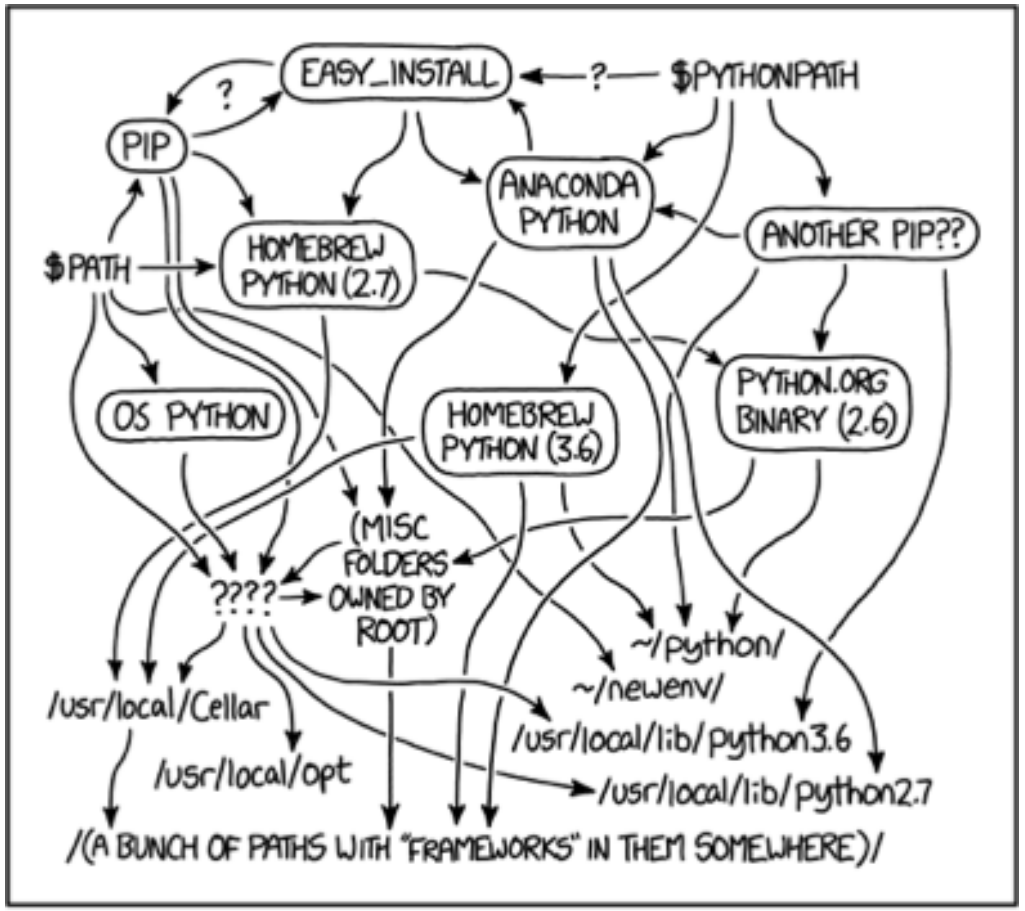
conda

What is a package manager

Software to automate process of installing, upgrading, configuring, removing, applications/programs in a consistent manner



Common Linux package mangers include apt, snap, ppa dpkg, yum, rpm etc.

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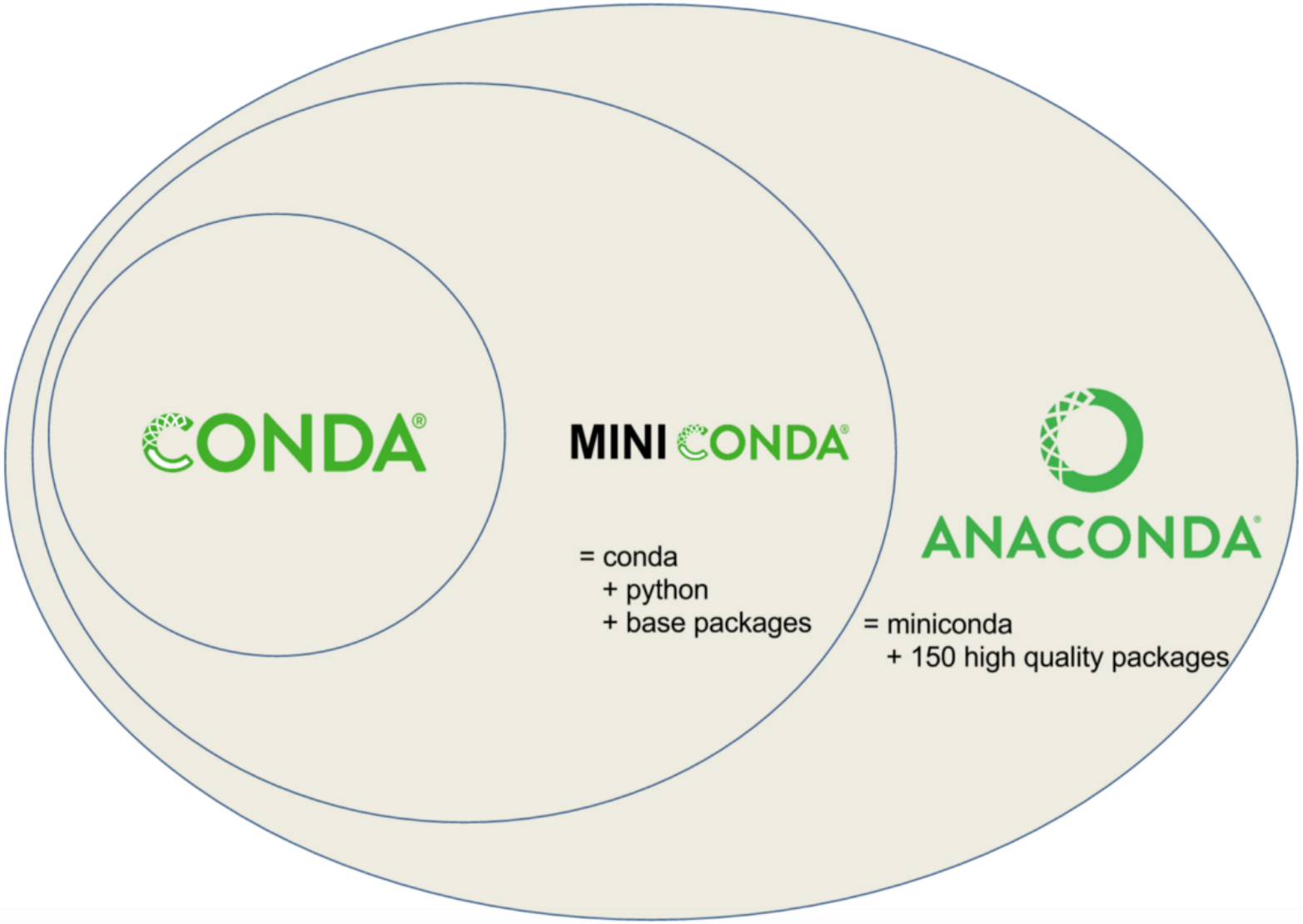
What is a package manager

Package, dependency and environment management for any language

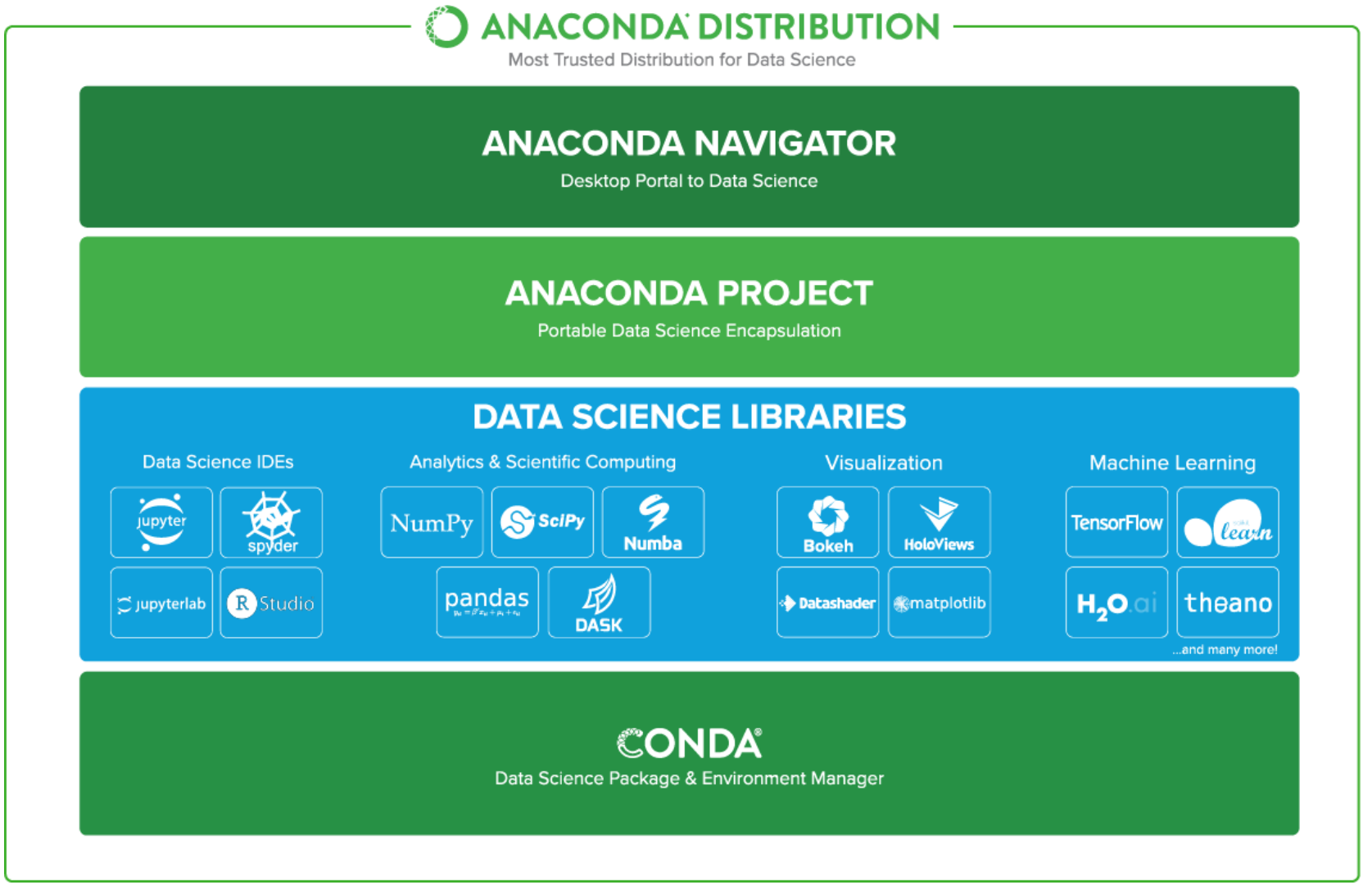
"Conda is an open source package management system and environment management system that runs on Windows, macOS and Linux. Conda quickly installs, runs and updates packages and their dependencies. Conda easily creates, saves, loads and switches between environments on your local computer. It was created for Python programs, but it can package and distribute software for any language."

from: https://conda.io/docs/

What is Miniconda / Anaconda?



What is Miniconda / Anaconda?



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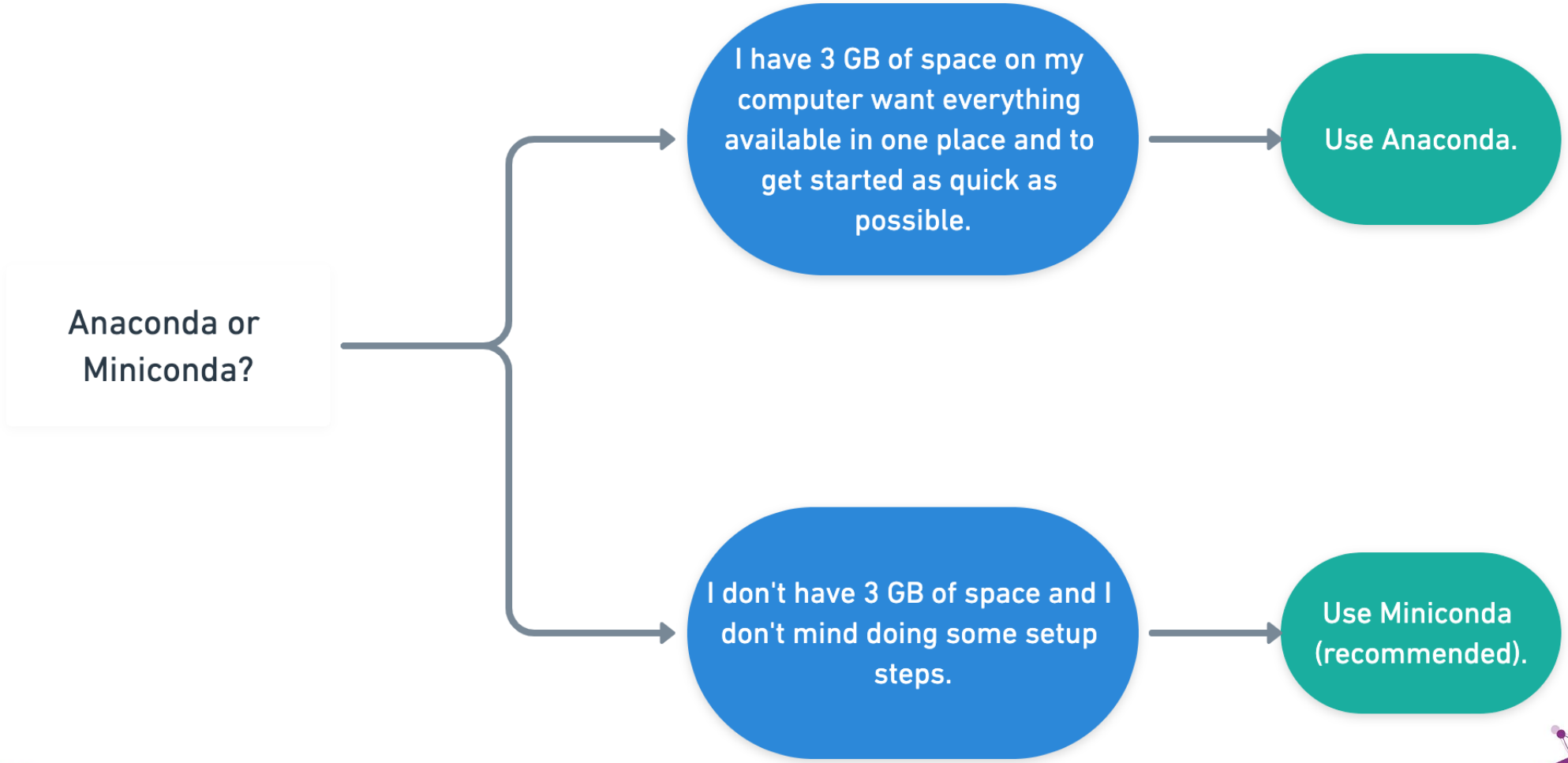
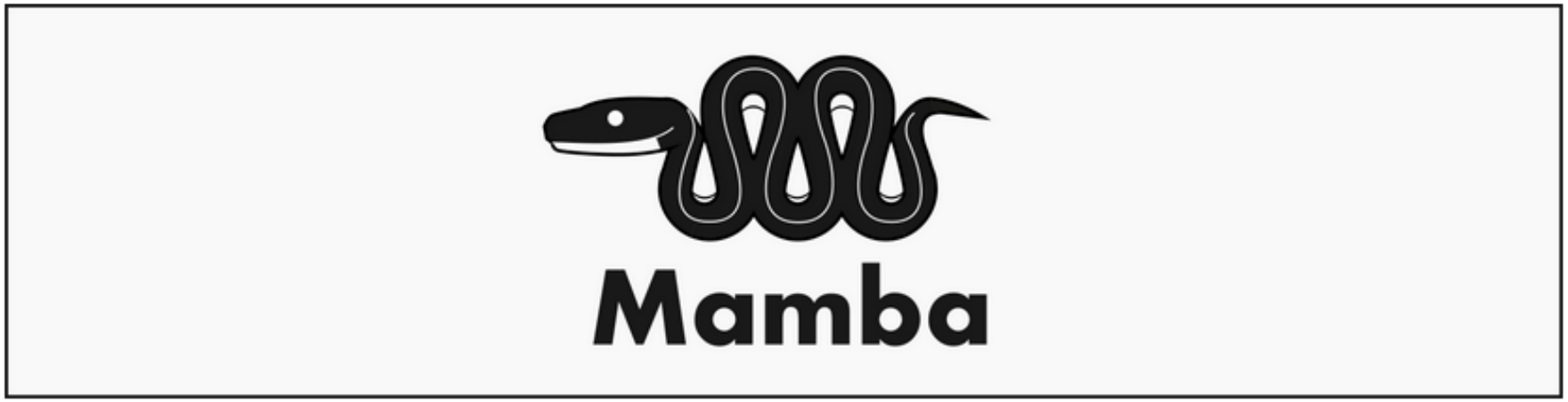
What is Miniconda / Anaconda?



What is Mamba?



The Fast Cross-Platform Package Manager

part of mamba-org		
Package Manager mamba	Package Server quetz	Package Builder boa

mamba

CI passing | gitter join chat | docs passing

`mamba` is a reimplementation of the conda package manager in C++.

Back up your data regularly !!!