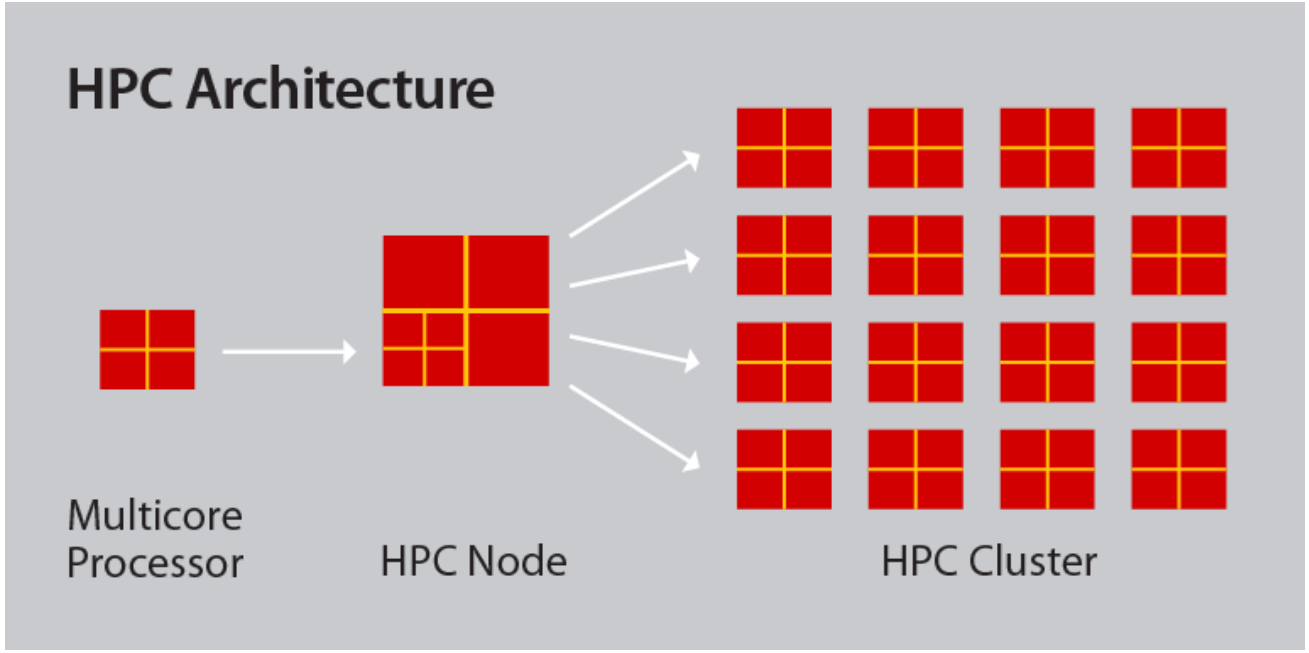
Summer of AI 2021: Introduction to HPCs

Presenter: Mr Aninda Saha

What are HPCs?

- **Definition:** A collection of many computing nodes, including CPUs and GPUs, that are connected by a fast interconnect
- **Basic components:**
  - Multiple computers
  - Connected over a network
  - With a shared file system
  - Supports running a parallel application across several computers
- Built-in modules can be accessed through `module avail`
- Does not provide sudo access so sometime maybe preferable to use miniconda to create virtual environments



What are HPCs used for?

Design Simulation

Molecular simulation for drug development

Design new materials with selected properties

Fundamental research

Synapse Modelling to understand how brain works

Simulations of the birth of the universe

Heavy computational workloads

Data analysis

Recommendations algorithms

Fraud detection for credit card

Optimization

Portfolio optimization in finance

Optimization of networks or storage of commodities

Behavior prediction

Prediction models for climate change

Predictive maintenance for industry

HPCs @ UQ

- **Goliath cluster (soon to be replaced by Rangpur cluster)**
  - Accessible to students and staff
  - Requires VPN to access from off-campus (https://my.uq.edu.au/information-and-services/information-technology/working-remotely/vpn-virtual-private-network)
  - https://student.eait.uq.edu.au/infrastructure/compute/
- **Wiener cluster**
  - Most resourceful HPC in the southern hemisphere
  - Serviced by the Research Computing Center (RCC) & Queensland Brain Institute (QBI)
  - Requires special access which can be attained by sending a request to helpdesk@qbi.uq.edu.au
  - https://rcc.uq.edu.au/wiener
- **Tinaroo, Flashlite and Awoonga clusters**
  - Similar concepts to Wiener and Goliath
  - https://rcc.uq.edu.au/high-performance-computing

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Summer of AI 2021: HPC Tips & Tricks

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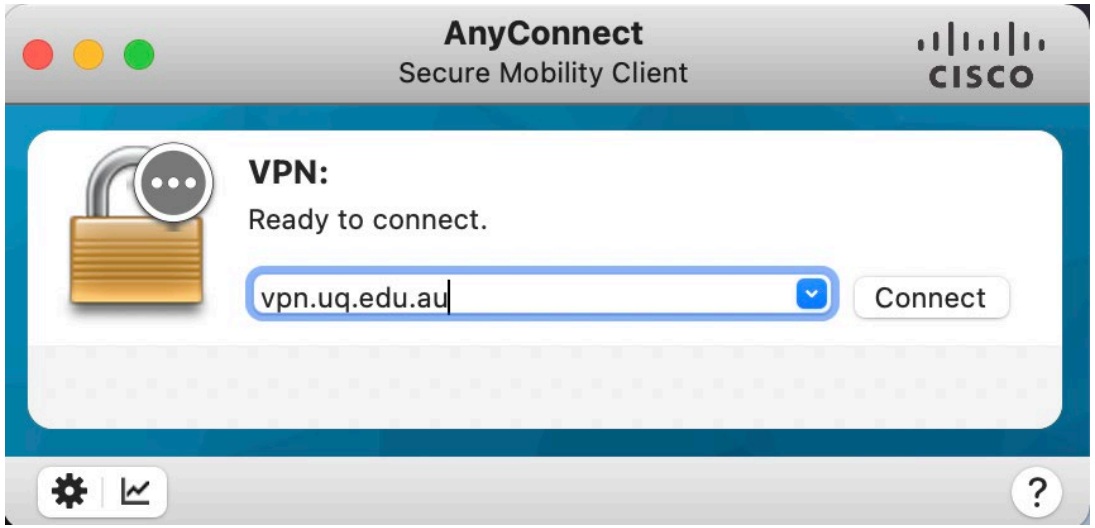
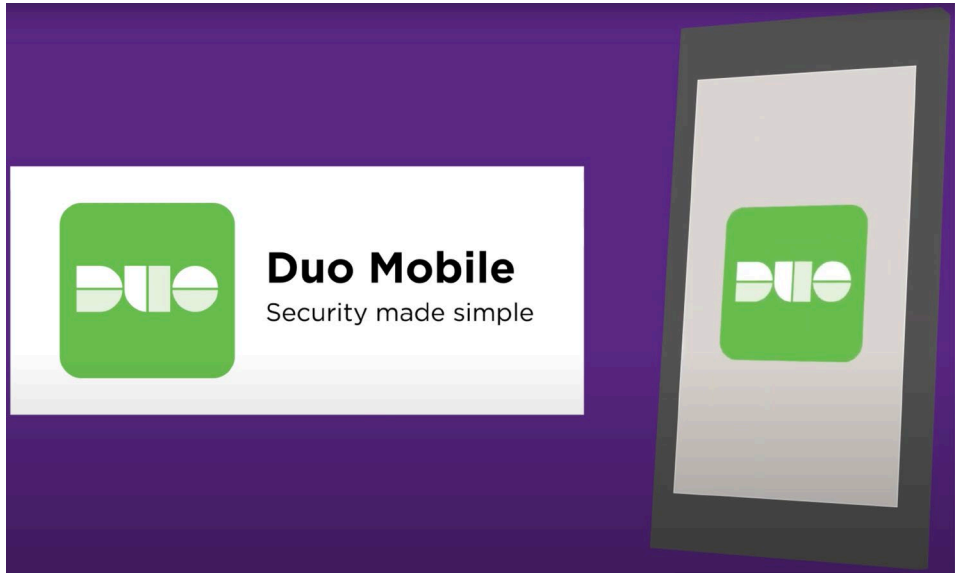
VPN Access (Goliath)

- Install AnyConnect Secure Mobility VPN Client from here (requires staff or student login): https://vpn.uq.edu.au/
- Launch client and connect to the UQ VPN at **vpn.uq.edu.au**



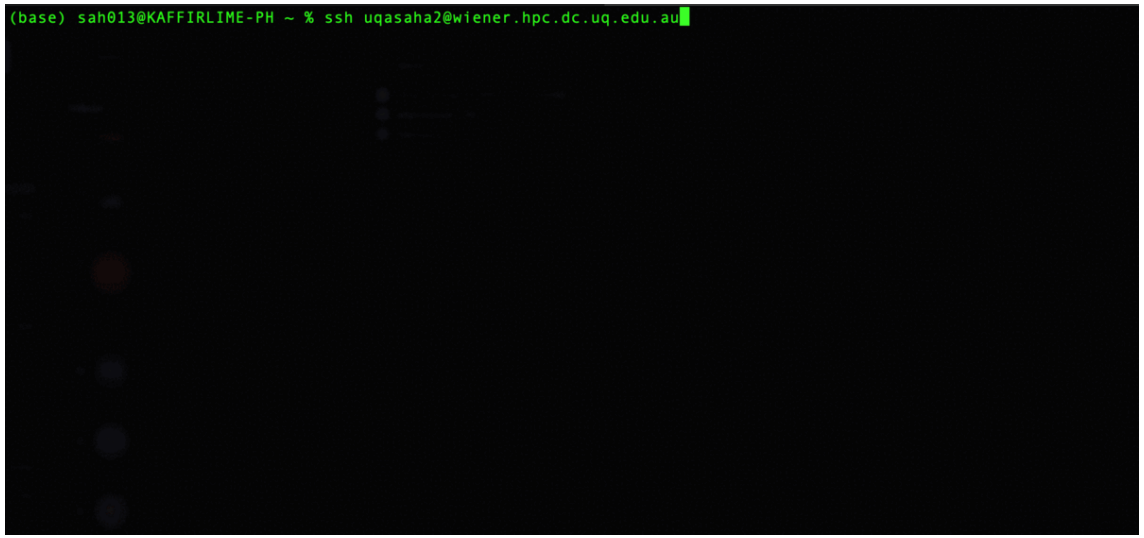
MFA (Wiener)

- Multi-factor authentication (MFA) now enabled for Wiener, so does not require VPN but requires registering with Duo Mobile authentication from: https://mfa.uq.edu.au/auth



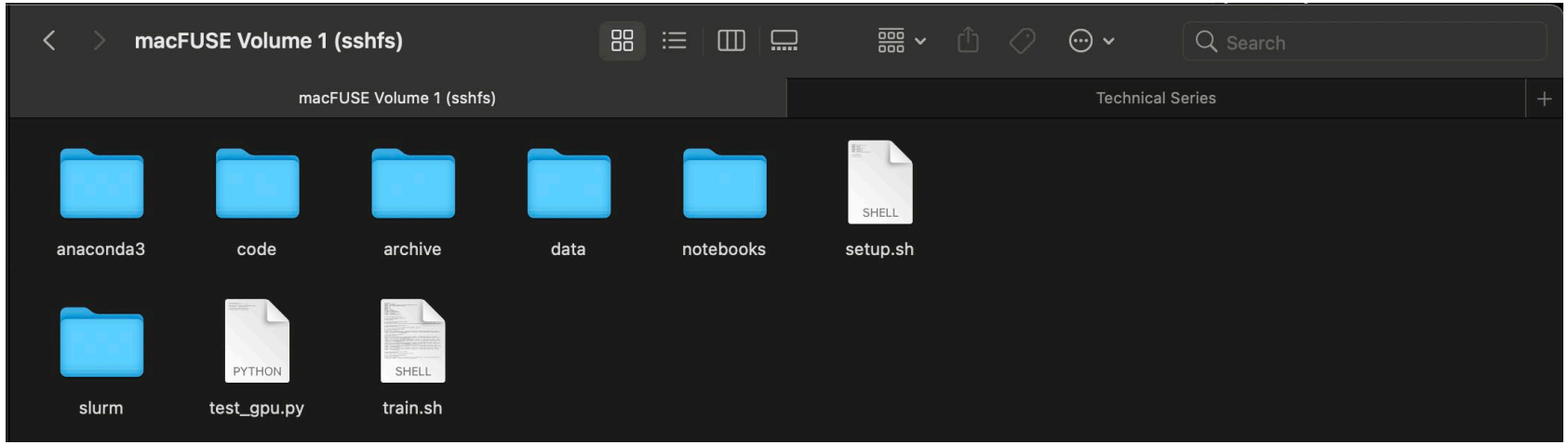
SSH Key for Quick Login

- Login to HPC shell using ***ssh sxxxxxx@hpc.uq.edu.au*** but this requires you to enter your password every time
- It can be helpful to setup SSH keys to login quickly without typing in your password every time. Follow these steps:
  - Type into **HPC terminal:**
    - `mkdir -p ~/.ssh` – creates directory for storing ssh key
    - `chmod 700 ~/.ssh` – restrict permissions of directory
  - Type into your **PC terminal:**
    - `ssh-keygen -t rsa` – generate the ssh key for your computer
    - `ssh-copy-id -i ~/.ssh/id_rsa.pub user@server` – copy ssh key to the HPC



SSHFS for File System Mount

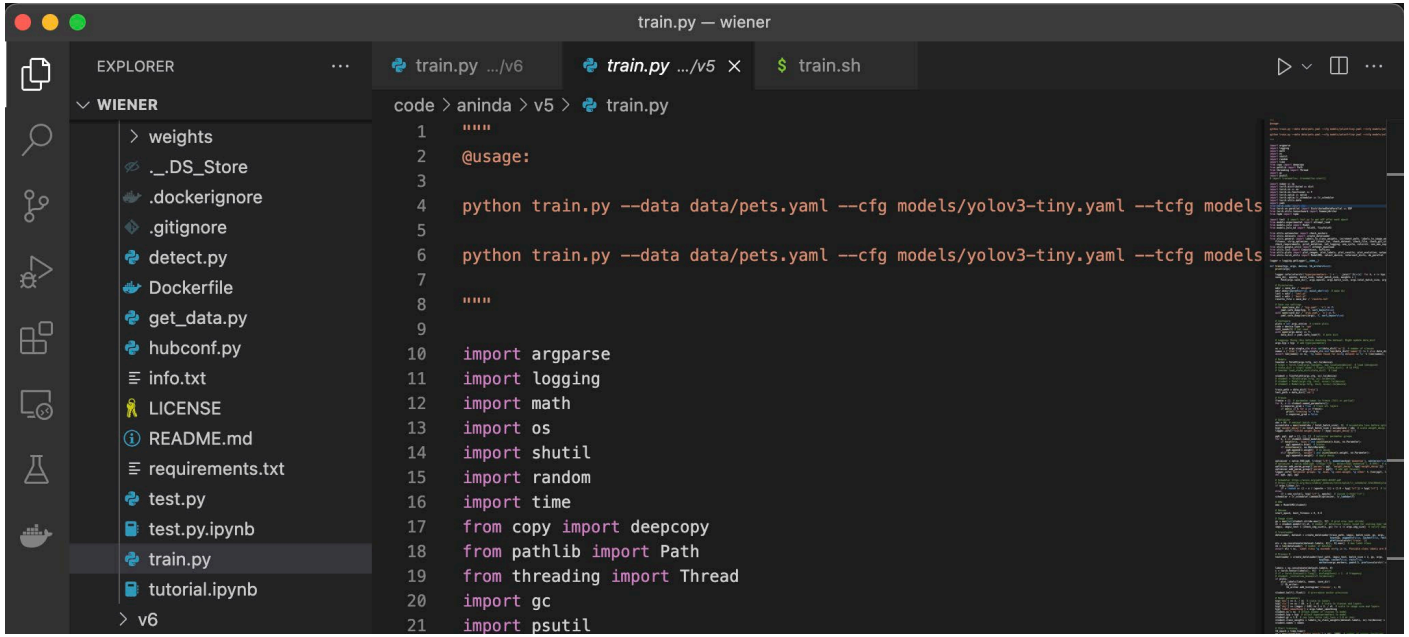
- While navigating the HPC through the terminal and editing with VIM/Nano can be fun, it can also be helpful to setup a filesystem mount locally which can allow editing code through VS Code
- To mount, type in on your **Linux or Mac terminal**:
  - `sshfs user@wiener.hpc.dc.uq.edu.au:/path/to/mount/on/HPC /local/mount/path`



- To unmount, type in on your **Linux or Mac terminal**:
  - `diskutil unmount force /local/mount/path`

Aliases

- Using aliases can cut down time having to type in these setup commands
- For easy login and file system mounting, use the following aliases:
  - `alias wiener="ssh -t user@wiener.hpc.dc.uq.edu.au 'cd /HPC/login/path; bash --login'"`
  - `alias wiener_fs="sshfs user@wiener.hpc.dc.uq.edu.au :/path/to/mount/on/HPC /local/mount/path; code /local/mount/path"`
  - `alias wiener_fsu="diskutil unmount force /local/mount/path"`



Navigating Wiener

- By default, logging in places you into the head node at `/clusterdata/user` which has a 5GB storage limit
- To access lots of data storage, use the scratch directory or the Research Data Manager (RDM) mount:
  - `/scratch/itee/user` – scratch directory
  - `/afm01 or /afm02` – RDM directory
- DO NOT run compute-intensive jobs on the head node
- Use Slurm to run training jobs, which will be discussed shortly by the next presenter

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Thank you

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