A very quick introduction to HPC

(HPC = High Performance Computing)

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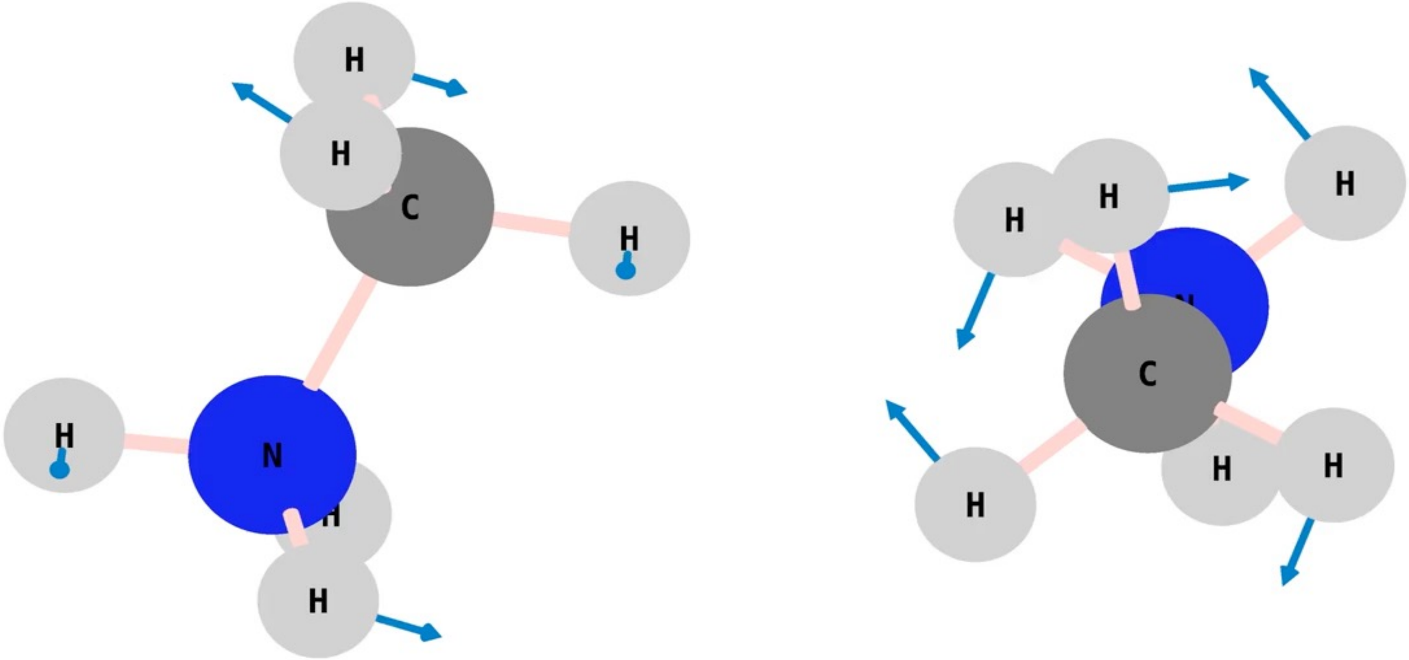
Who am I?

- My name is Dr Lucy Whalley
- Vice-Chancellor’s Fellow in Physics at Northumbria
- Member of the EE Faculty HPC steering group
- I use HPC for my research in solid-state physics

(HPC = High Performance Computing)

Quantum mechanical vibrations



Courtesy Jarvist M. Frost

OUTLINE

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02 HPC basics

03 Finding out more

04 Questions

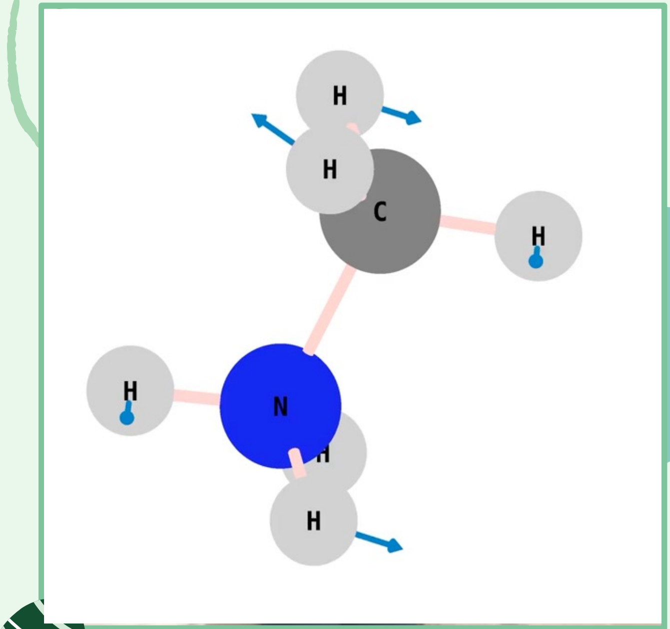
Why use HPC?

Research problems can outgrow the computer where they started

- Statistical validation – running the same model 1000 times, each time takes an hour
- Increase in dataset size – the new data is 10 times as large and will crash a laptop
- Increase in model complexity – going from 2D to 3D simulations leads to a large increase in simulation time

Supercomputers (also known as clusters) are optimized for intensive computing

This calculation would take 24 days on my laptop (and would really slow down ~~Netflix~~ Teams meetings)



Why use HPC?

Using a cluster has several advantages

- **Speed** – clusters have ***lots of*** cores
- **Volume –** processing memory (RAM) and disk storage for large amounts of data
- **Efficiency –** as there are many system users
- **Cost** – bulk purchasing results in a reduction in cost
- **Convenience** – why tie up your own computer for hours if you can use another one?

02

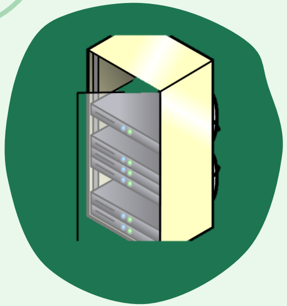
HPC basics

What is a supercomputer?

What is a supercomputer?

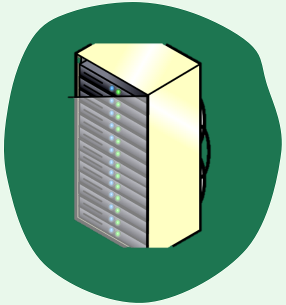
Laptop

2 cores



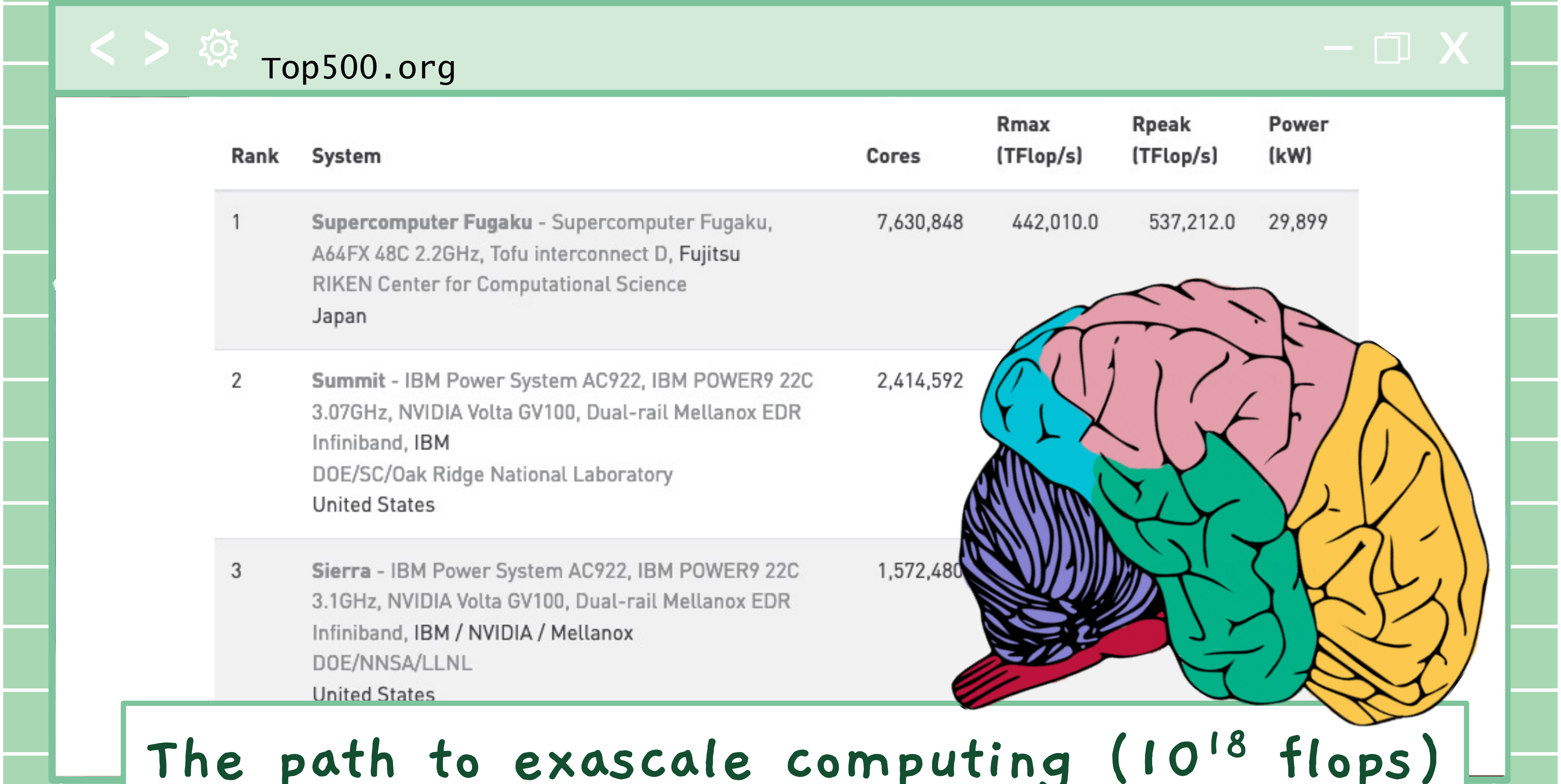
Server

16-128 cores



Supercomputer

~500 – 7.6 million cores



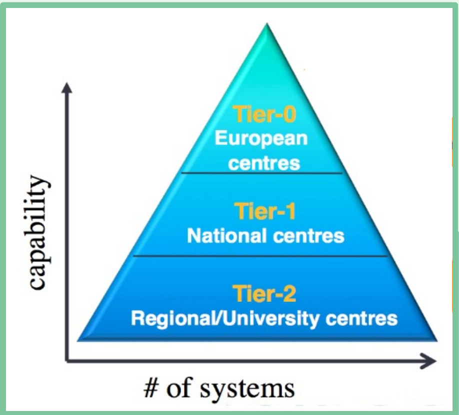
Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592			
3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480			

The path to exascale computing (10^{18} flops)

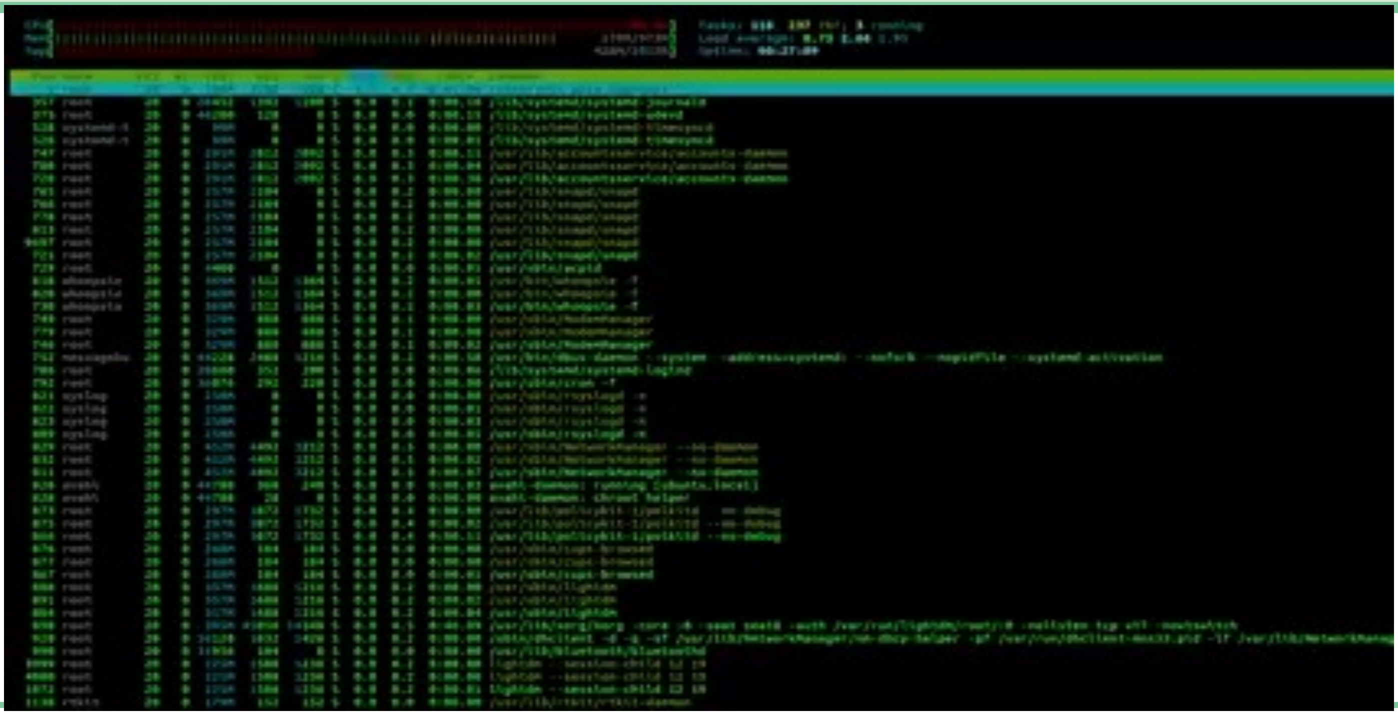
Which computers can I access?

HPC facilities are structured according to tiers

TIER	COMPUTER	Access route
0	Multiple	Prace - (http://prace-ri.eu)
1	Archer2	Multiple
2	Oswald	Raise an IT ticket

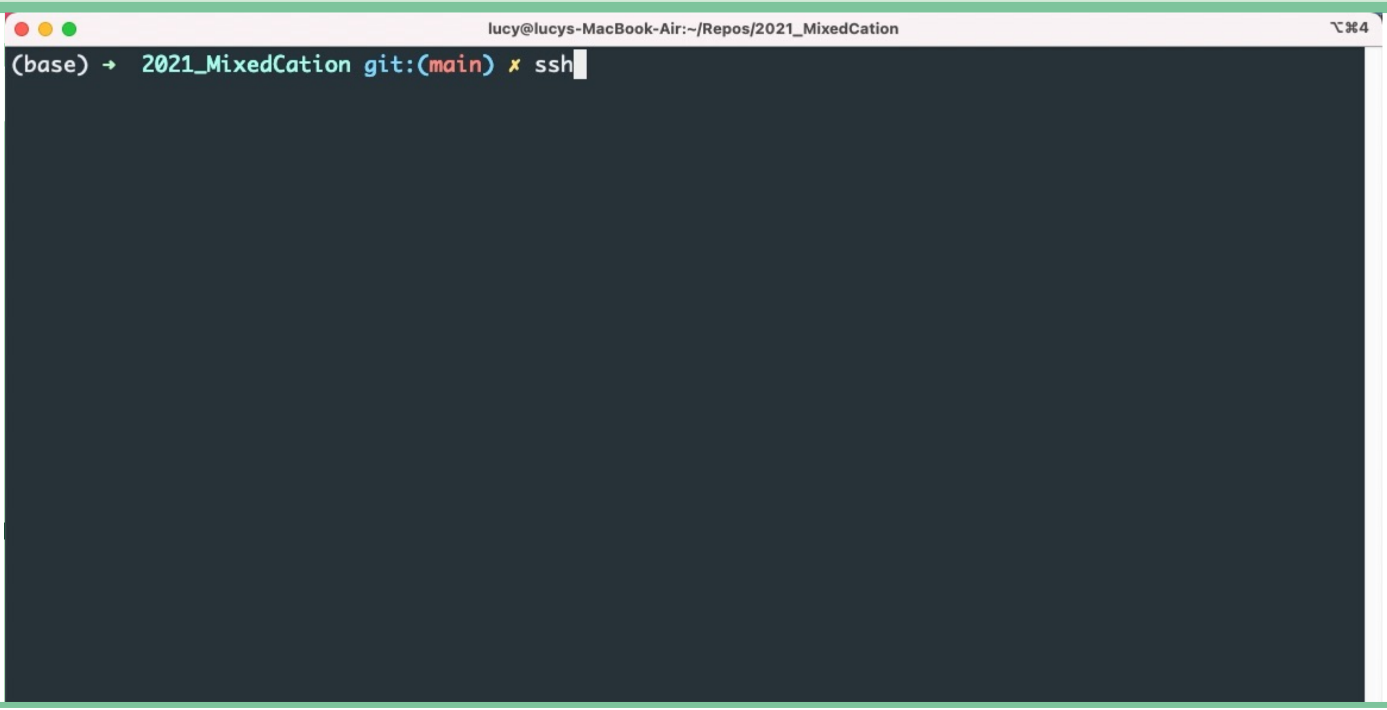


How do I access the computer?



Using a terminal (just like the movies)

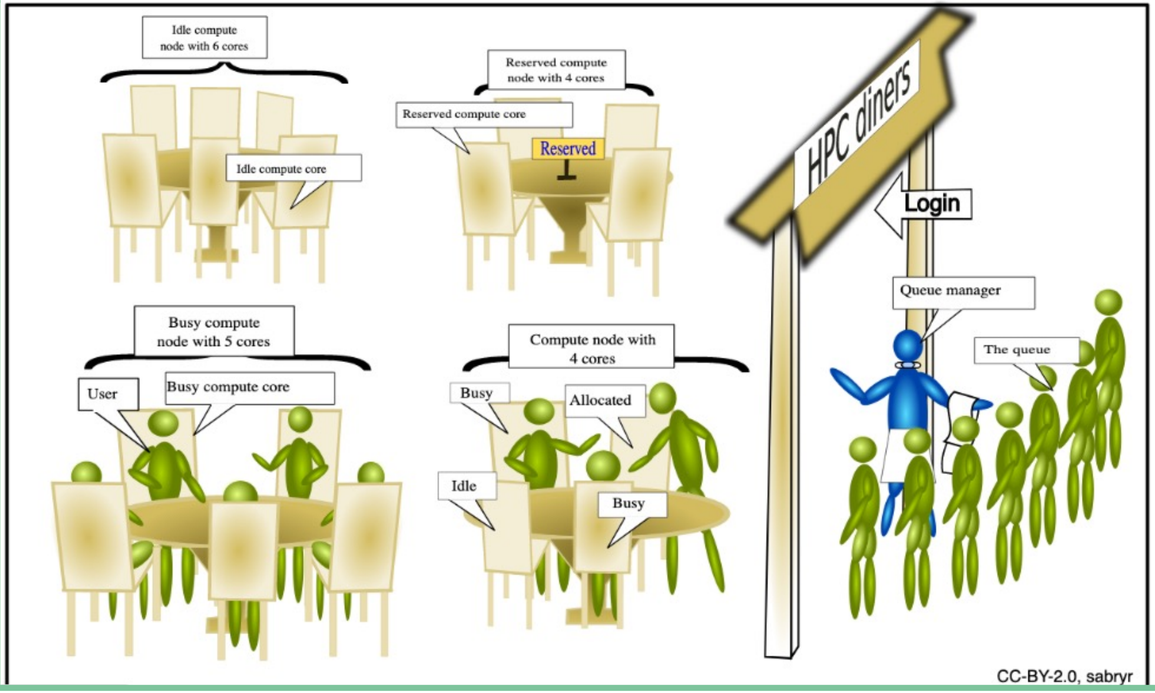
How do I access the computer?



```
(base) ➜  2021_MixedCation git:(main) ✗ ssh
```

Using a terminal and Unix commands

How are resources distributed?



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A schedular is used to manage the job queue

03

Finding out more

What next?

Where can I get more support?

Departmental HPC rep

MCE: Craig Warren

RSE community rep

Lucy Whalley

To access Oswald

Raise an IT Ticket

Archer2 national cluster

www.archer2.ac.uk

HPC workshops

www.archer2.ac.uk
/training/

PRACE European cluster

https://prace-ri.eu/

THANKS!

slides: `lucydot.github.io/talks`

Watch out for the Research Software Engineering @ Northumbria event this autumn

Credits: Slidesgo, Flaticon, Freepik,
epcced.github.io/hpc-intro-2020-06-30/