

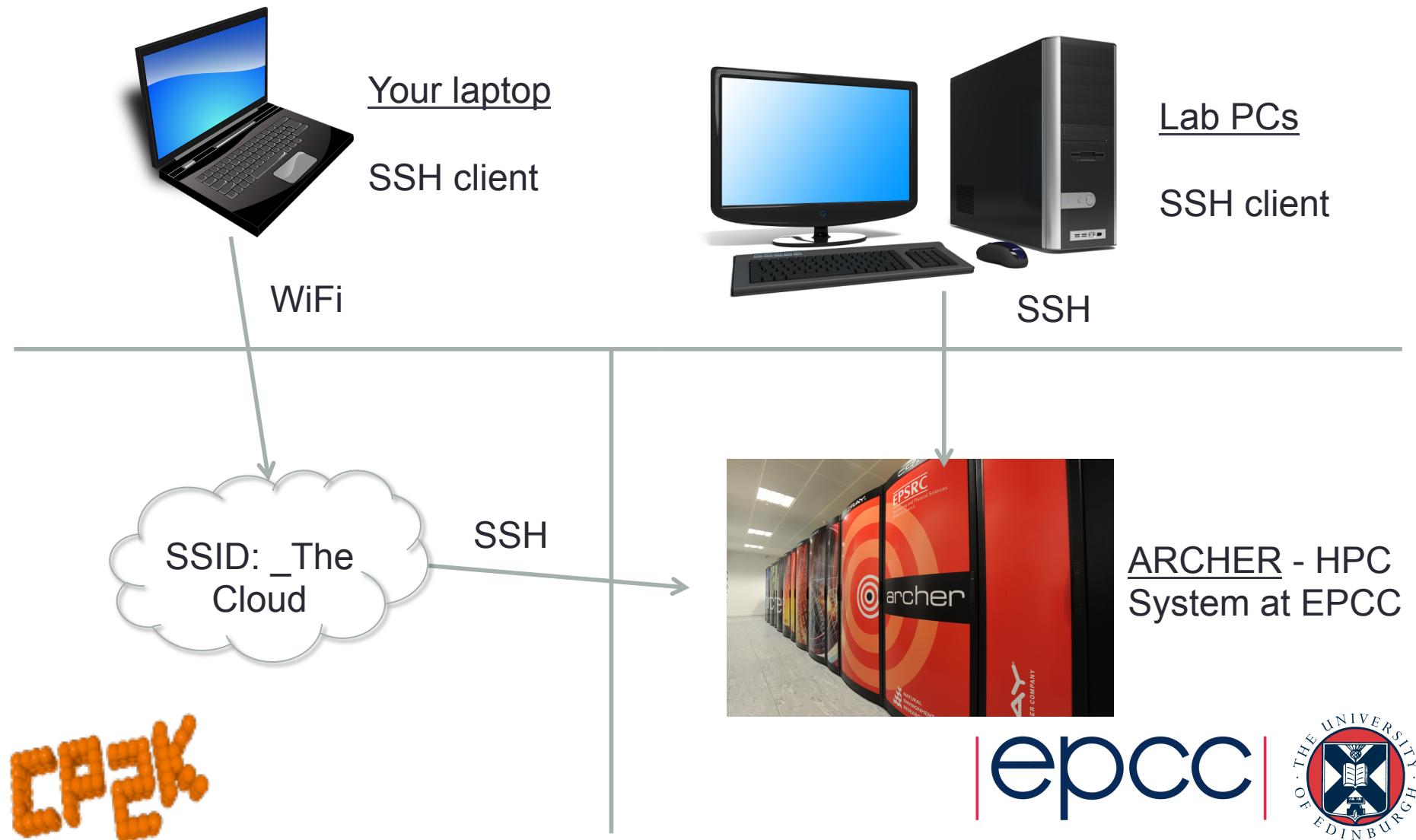
SETTING UP COMPUTER ACCOUNTS

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Overview – Infrastructure



CP2K

Where to run CP2K?

- Own Laptop
 - Serial / OpenMP build
- Your own institute workstation / cluster
- KCL Guest logins
 - CP2K 3.0 pre-installed
- ARCHER Guest accounts
 - Cray XC30 @ EPCC
 - CP2K 3.0 psmf pre-installed, massively parallel calculations



CP2K

| epcc |



ARCHER in a nutshell

- UK National Supercomputing Service
 - £43 million 4-year project from 2013
- Cray XC30 Hardware
 - Nodes based on 2×Intel Ivy Bridge 12-core processors
 - 64GB (or 128GB) memory per node
 - 4920 nodes in total (118080 cores)
 - Linked by Cray Aries interconnect (dragonfly topology)
 - Linpack performance 1.64 PFLOP/s (#40 on Top500)
- Managed by EPSRC
 - Operated, housed and supported by EPCC



ARCHER Guest Accounts

- All participants are allocated a guest account:
 - Pick up sign-up sheet which has your username on it
 - `ssh guestXXX@login.archer.ac.uk` to log in
- Accounts will be available until 26th August, when they will be locked and erased
 - Copy any data back to your home institution before then
- Guest accounts are part of group `y14`
 - This is the budget you will use to run jobs



ARCHER Reservations

- Guest accounts may submit jobs at any time
 - Queue waiting time may be several hours
- Reservations allow your jobs to bypass the queue and run (almost) instantly
 - Subject to the other users on the course sharing resources fairly!
 - 50 ARCHER nodes are reserved (1200 cores)
- To use the reservation you need to specify the reservation ID `“course1”`



ARCHER Reservations

- Reservation queue is open:
 - 16:00-17:00 Tuesday 23rd
 - No reservation on Wednesday – ARCHER ‘at risk’ maintenance
 - 11:15-13:00 Thursday 25th
 - 15:15-17:00 Thursday 25th
 - 11:15-13:00 Friday 26th
- Outside these times (overnight) omit the reservation ID to submit to the normal queue
- Need help with ARCHER?
 - See <http://www.archer.ac.uk/documentation>
 - Ask us!

