



Hartree Centre

Science & Technology Facilities Council

# SETTING UP COMPUTER ACCOUNTS

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# Overview – Infrastructure



Your laptop

SSH client

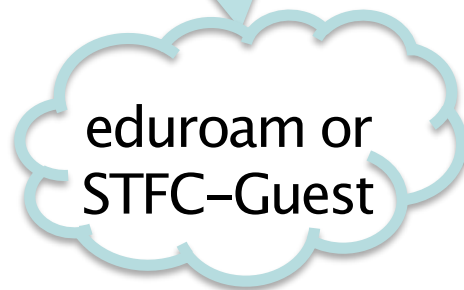


Lab PCs

SSH client

WiFi

SSH



SSH



ARChER – HPC  
System at EPCC

CP2K



# Where to run CP2K?

- Own Laptop
  - Serial / OpenMP build
- Your own institute workstation / cluster
- ARCHER Guest accounts
  - Cray XC30 @ EPCC
  - CP2K 6.1 psmf pre-installed
  - Parallel calculations (MPI)



CP2K



# ARCHER in a nutshell

- UK National Supercomputing Service
  - £43 million, installed in 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 (#79 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 22<sup>nd</sup> June, 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!
  - 25 ARCHER nodes are reserved (600 cores)
- To use the reservation you need to specify the reservation ID with  
“`qsub -q Rxxxxxxx`”





# ARCHER Reservations

- Reservation queue is open:
  - R5390913: 13:00-17:00 Tuesday 19<sup>th</sup>
  - R5390920: 09:00-17:00 Wednesday 20<sup>th</sup>
  - R5390921: 09:00-17:00 Thursday 21<sup>st</sup>
  - R5390924: 09:00-13:00 Friday 26<sup>th</sup>
- 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!

