



Hartree Centre

Science & Technology Facilities Council

SETTING UP COMPUTER ACCOUNTS

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CP2K



Overview – Infrastructure



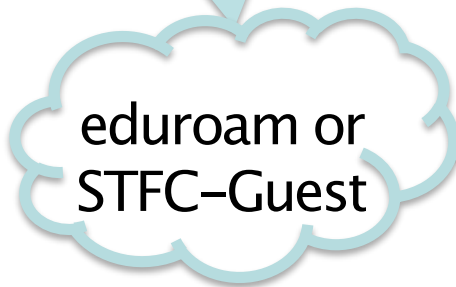
Your laptop
SSH client



Lab PCs
SSH client

WiFi

SSH



eduroam or
STFC-Guest

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 22nd 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 19th
 - R5390920: 09:00-17:00 Wednesday 20th
 - R5390921: 09:00-17:00 Thursday 21st
 - R5390924: 09:00-13:00 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!

