SETTING UP COMPUTER ACCOUNTS

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Overview – Infrastructure

Your laptop
SSH client

Lab PCs
SSH client

WiFi

eduroam or STFC-Guest

SSH

ARCHER – HPC System at EPCC
Where to run CP2K?

• Own Laptop
  • Serial / OpenMP build

• Your own institute workstation / cluster

• ARCHER Guest accounts
  • Cray XC30 @ EPCC
  • CP2K 6.1 psmp pre-installed
  • Parallel calculations (MPI)
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\textsuperscript{nd} 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!