SETTING UP COMPUTER ACCOUNTS

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Overview – Infrastructure

- Your laptop
  - WiFi
  - SSH client

- Lab PCs
  - SSH

- SSID: _The Cloud

- ARCHER - HPC System at EPCC
  - epcc
  - 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 psmp pre-installed, massively parallel calculations
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!