An Introduction to High Performance Computing

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Research Computing Services (http://www.hpc.cam.ac.uk/)
University Information Services (http://www.uis.cam.ac.uk/)

30th July 2019 / UIS Training

Welcome

- Please sign in on the attendance sheet.
- Keep your belongings with you.
- Please ask questions and let us know if you need assistance.

UIS: Research Computing Services

Your trainers for today will be:

▶ Paul Sumption
          Research Computing User Services

▶ Eleftherios Avramidis
          Research Software Engineering

You may be . . .

- ▶ Programmers (or not).
- ▶ UNIX power users (or not).
- ▶ Researchers wishing to run large, parallel code.
- ▶ Researchers wishing to run many, non-parallel cases.
- ▶ Researchers interested in big data, machine learning, AI.
- ▶ Researchers requiring slightly more than an ordinary workstation.
- ▶ Many different disciplines and requirements.

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Plan of the Course

Part 1: Basics
Part 2: Research Computing Services HPC
Part 3: Using HPC

10:00	WELCOME
11:00-11:15	Break
12:30-13:30	LUNCH
15:30-15:45	Break
16:30	CLOSE

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Topics Covered

• Hardware

• Storage

• Access

• Data Transfer

Hardware

- Gateway or Bastion hosts (bslcenb & bslce
    - Only use for access to BAS or transferring fil
- Headnodes
    - No access, manages job queues and storage
- General Use Workstations & Private W

Access

Authentication

- â¢ Three passwords â UNIX (NIS), LDAP and S
- â¢ UNIX for bslcenb /bslcenc and LDAP for HP
- â¢ Try to keep all these password synchronised
- â¢ We are working to simplify the situation

SSH

Access (continued)

X2Go

- â¢ Access HPC desktop interface with or witho

- â¢ Disconnecting and reconnecting

- â¢ Copy/paste

- â¢ Sharing files from your laptop or PC

- â¢ More information: http://ictdocs/wiki/index.p

Storage

User Area - /users/username

- Small, not intended for sharing data

- Space restricted via quotas

SAN Volumes

- Setup for projects and departments, eg: : /da

- Accessible from workstations, hslcsnb, hslcs

Storage (continued)

HPC Storage - /data/hpcdata/ (users, dat

  â¢ Accessible from nodes and workstations, bsl

  â¢ Usage limited via quotas

Quotas

  â¢ On HPC you can check your quotas using: m

  â¢ Need more space - contact the service desk

Data Access and Transfer

Samba

- â¢ Allows clients to connect to UNIX storage as

- â¢ Allows access to SAN volumes, /users and /

- â¢ No access to /data/hpcflash

FTP

- â¢ Allows non-RAS users to retrieve files from th

Data Access and Transfer(o

- rsync

    - Perfect tool for transferring file locally and s

    - Options to resume, reconnect, compression

- scp

- sshfs

UserEnvironment

â¢Shell

- â¢ Our default shell is tcsh

- â¢ If you prefer something different such as bas

â¢SSH keys

- â¢ Connect to BAS systems without typing pass

- â¢ ssh-keygen ê Always create with a passphra

UserEnvironment

- tmux

  - Keeps long running command line sessions
  - Allows disconnecting and reconnecting
  - Multiple command line sessions and console
  - More information: http://ictdocs/wiki/index.php
  - Demonstration

Software

Operating System software

- â¢ Typical linux commands and some graphica

- â¢ These can be run from the command line a

Modules

- â¢ Do not work on bslcenb or bslcenc

- â¢ There are two module repositories: /packag

Software (continued)

Modules

- â¢ Useful module commands:

    module avail

    module load name/version

    module unload name/version

- â¢ Common mistakes

JupyterNotebooks

â¢Jupter notebooks running on workstatio

â¢More information: http://ictdocs/wiki/in

Containers

- Containers at BAS are still a work in pr

- What are containers?

- Podman

  - To be able to use, you need to contact the se

  - Container images must be downloaded to ea

S LURM

- What is it?
  - Simple Linux Utility for Resource Manageme
  - Schedules jobs based on the resources they
- Different queues
  - Short -
  - Medium

SLURM

Job Types

- Batch â Standard job

- MPI

  - When you require large amounts of memory or cpu cores

  - MPI require infiniband connectivity for Messaging

  - All nodes need to be in the same queue.

SLURM (continued)

â¢Job submission scripts â Simple:

SLURM (continued)

• Job monitoring

  • squeue -u <username>

  • sacct -j <jobid>

  • To see details on resources used by all runni

  • To see all your recent jobs: sacct -u <usernam

  • To check memory and cpu usage on a node:

SLURM (continued)

- Troubleshooting failed jobs

    - Set an output file, often has useful informatio

- Common mistakes

    - Forgetting to load modules

    - Using storage which is not visible to the HPC

    - Avoid using symlinks

Model Ensembler

â¢Aimed at solving complex HPC worklo

Developer Environment

â¢Use git!

â¢Repeatable, reproducible & shareable

BestPractice

- User Policy

    - Link:

- Do!

    - Ask for help,

- Don't!

HELP!

- Service desk: servicedesk@bas.ac.uk

- HPC User Guide: http://ictdocs/wiki/inc

- Service Desk Solutions

- Yammer

Any Que

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