



An Introduction to High Performance Computing 2021

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December 16, 2021



Welcome

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

BAS: HPC Computing Services

Your trainers for today will be:

- ▶ **Paul Sumption**
HPC Engineer
- ▶ **Andrew England**
HPC service owner



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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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Part I

Basics

Basics: Topics Covered

- ▶ Hardware
- ▶ Storage
- ▶ Access
- ▶ User Environment
- ▶ Software
- ▶ Containers
- ▶ SLURM
- ▶ Model Ensembler
- ▶ Best Practise
- ▶ HELP!



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Access: Hardware

- ▶ Gateway or Bastion hosts (bslcnb & bslcnc)
 - ▶ Only use for access to BAS or transferring files, donât use for running programs
- ▶ Headnodes
 - ▶ No access, manages job queues and storage (/data/hpcdata)
- ▶ General Use Workstations Private Workstations
- ▶ Nodes
- ▶ GPU Nodes
 - ▶ Currently only available for use BAS AI Lab members
- ▶ Development Workstation and Development Node
 - ▶ No access, used for testing by IT



Authentication

- ▶ Three passwords: UNIX (NIS), LDAP and Samba
- ▶ UNIX for bsicenb / bsicenc and LDAP for HPC workstations
- ▶ Try to keep all these password synchronised
- ▶ We are working to simplify the situation



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SSH

- ▶ First connect to gateway hosts: `bslcnb.nerc-bas.ac.uk` / `bslcenc.nerc-bas.ac.uk`
- ▶ Second connect to HPC workstations: `bslws01` â `bslws12`
- ▶ OpenSSH (available for Linux, Mac windows), Putty, WSL, MobaXterm

Demonstration



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- ▶ Access HPC desktop interface with or without VPN access
- ▶ Disconnecting and reconnecting
- ▶ Copy/paste
- ▶ Sharing files from your laptop or PC
- ▶ More information: <http://ictdocs/wiki/index.php/HPC:X2GO>
- ▶ **Demonstration**



x2go alternatives

- ▶ Exceed / Xming
- ▶ MobaXterm
- ▶ **Demonstration**



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Storage

User Area - `/users/username/`

- ▶ Small, not intended for sharing data
- ▶ Space restricted via quotas
- ▶ Not accessible from the HPC Nodes!

HPC Storage - `/data/hpcdata/users/username`

- ▶ Accessible from nodes and workstations, bsfcenb, bsfcenc.
- ▶ Usage limited via quotas



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Storage SAN Volumes

- ▶ Setup for projects and departments, eg: : */data/cruise, /data/vlf*
- ▶ Accessible from workstations, bsicenb, bsicenc
- ▶ Volume should be managed and curated by a data manager
- ▶ Space is not controlled by quota's
- ▶ Adding additional space depends availability of physical disk space
- ▶ Contact data manager first if you think you require additional storage



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Storage policies

Quotas

- ▶ On HPC you can check your quotas using: myquota
- ▶ Need more space - contact the service desk

Backups

- ▶ Daily at 6pm
- ▶ All SAN and HPC volumes backed up
- ▶ Backups are both onsite and offsite, via tapes disk
- ▶ If you need a file restored, contact the service desk



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Data access

Samba

- ▶ Allows clients to connect to UNIX storage as if it were a windows network share.
- ▶ Allows access to SAN volumes, /users and /data/hpcdata
- ▶ No access to /data/hpcflash



SFTP

SFTP

- ▶ Allows non-BAS users to retrieve files from the FTP area
`ftp://ftp.bas.ac.uk/`
- ▶ Users within BAS can gain access to this area and deposit files
- ▶ Please contact the IT ServiceDesk to have a directory setup
ie. `/data/ftp/username`

Writeable FTP Area

- ▶ Possible for non-BAS users to upload files as well, please contact the IT ServiceDesk for details



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Data access (continued)

rsync

- ▶ Perfect tool for transferring file locally and securely over the internet
- ▶ Options to resume, reconnect, compression, limit transferred rates.

scp

sshfs



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Part II

User Environment

User Environment

Shell

- ▶ Shell
- ▶ Our default shell is tcsh
- ▶ If you prefer something different such as bash, contact the service desk



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SSH Keys

- ▶ SSH keys
- ▶ Connect to BAS systems without typing passwords
- ▶ ssh-keygen â Always create with a passphrase
- ▶ ssh-agent
- ▶ ./ssh/config
- ▶ More information: http://ictdocs/wiki/index.php/SSH_keys

Demonstration



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TMUX

- ▶ Keeps long running command line sessions running
- ▶ Allows disconnecting and reconnecting
- ▶ Multiple command line sessions and console splitting
- ▶ More information: <http://ictdocs/wiki/index.php/tmux>

Demonstration



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System Software

- ▶ Typical linux commands and some graphical packages are installed as part of OS.
- ▶ These can be run from the command line and desktop interface



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The Module System

- ▶ Do not work on bsfcenb or bsfcenc
- ▶ There are two module repositories: /packages/modules
/hpcpackages/modules
- ▶ Prefer /hpcpackages/modules - works with nodes and workstations
- ▶ Modules sometimes include the compiler used in their name
eg. hpc/netcdf/intel/4.4.1.1
- ▶ Works by adjusting shell variables eg. PATH,
LD_LIBRARY_PATH Loaded modules only affect the terminal you loaded them in



Modules: useful commands

- ▶ module avail
- ▶ module load name/version
- ▶ module unload name/version
- ▶ module display name/version
- ▶ module list
- ▶ module purge



Common mistakes

- ▶ Forgetting to use hpc modules on nodes
- ▶ Mixing modules created using different compilers
- ▶ Loading clashing modules
- ▶ More information:
http://ictdocs/wiki/index.php?title=HPC:User_Guide

Demonstration



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Jupyter Notebooks

- ▶ Jupyter notebooks running on workstations:
<http://jupyterhub.nerc-bas.ac.uk>
- ▶ More information:
<http://ictdocs/wiki/index.php/HPC:JupyterHub>



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Containers

Containers at BAS are still a work in progress

- ▶ What are containers?

Podman

- ▶ To be able to use, you need to contact the service desk
- ▶ Container images must be downloaded to each node or workstation



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Containers (cont)

Singularity

- ▶ Designed with HPC usage in mind
- ▶ Ready to use on workstations and nodes
- ▶ For more information:
<http://ictdocs/wiki/index.php/HPC:Containers>
- ▶ **Demonstration**



Part III

SLURM

SLURM

- ▶ What is it?
- ▶ Simple Linux Utility for Resource Management â our HPC resource manager
- ▶ Schedules jobs based on the resources they need



SLURM: Queues

Queues

- ▶ Short -
- ▶ Medium -
- ▶ Long -
- ▶ GPU -



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SLURM fair share

Fair Usage

- ▶ Ensures each user gets fair usage of each HPC queue
- ▶ Adjusts priorities of submitted jobs based on previous usage



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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.
- ▶ Array â When you want to run upto a 1000 small jobs
- ▶ GPU - To use GPU's you must include the âgres option with the number of GPU's you require: *SBATCH -gres=gpu:2*



SLURM: job script

Sample job script.....

Useful Options

- ▶ *Exclusive node:SBATCH -exclusive*
- ▶ *Specific node:SBATCH -nodelist=node022*



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SLURM: Job monitoring

- ▶ `squeue -u username`
- ▶ `sacct -j jobid`
- ▶ To see details on resources used by all running jobs: `scontrol show jobid add jobid`
- ▶ To see all your recent jobs: `sacct -u username`
- ▶ To check memory and cpu usage on a node: `scontrol show node inode`



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SLURM: Troubleshooting

- ▶ Set an output file, often has useful information when jobs fail
- ▶ Did you load any require modules
- ▶ Check your quota



Common mistakes

- ▶ Forgetting to load modules
- ▶ Using storage which is not visible to the HPC nodes (use either /data/hpcdata or /data/hpcflash)
- ▶ Avoid using symlinks
- ▶ More information:
http://ictdocs/wiki/index.php?title=HPC:User_Guide



Model Ensembler

- ▶ Aimed at solving complex HPC workloads.



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Developer Environment

- ▶ Use git!
- ▶ Repeatable, reproducible shareable - containers can help



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Best Practice

- ▶ User Policy
- ▶ Link:
- ▶ Do! Ask for help,
- ▶ Don't! Submit jobs which use more than 4 nodes at a time.



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HELP!

- ▶ Service desk: servicedesk@bas.ac.uk
- ▶ HPC User Guide:
http://ictdocs/wiki/index.php?title=HPC:User_GuideServiceDeskSolution
- ▶ Yammer
- ▶ Email List



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Any questions?



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