POLAR SCIENCE
FOR PLANET EARTH

An Introduction to High Performance Computing 2021

Paul Sumption
pasump@bas.ac.uk

December 16, 2021

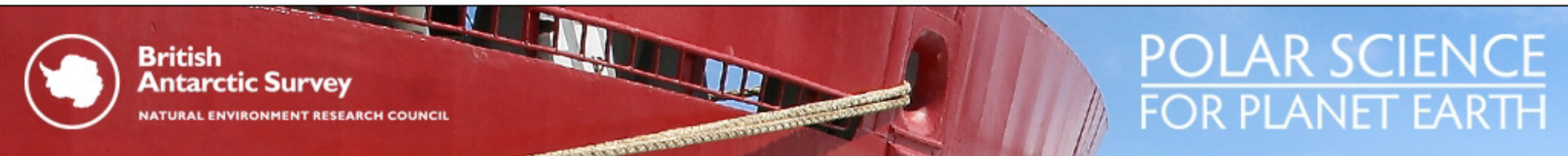
Welcome

- 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



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.**

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

Part I

Basics

Basics: Topics Covered

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

Access: Hardware

- Gateway or Bastion hosts (bslcenb bslcenc)
  - 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 â UNIX (NIS), LDAP and Samba
- UNIX for bslcenb / bslcenc and LDAP for HPC workstations
- Try to keep all these password synchronised
- We are working to simplify the situation

SSH

- First connect to gateway hosts: bslcenb.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

x2go

- 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

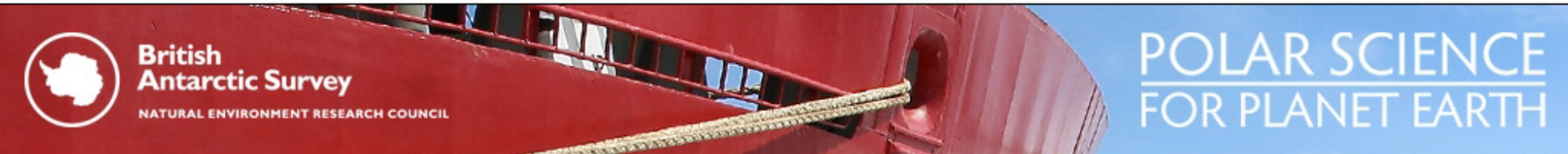
Storage

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, bslcenb, bslcenc.
- Usage limited via quotas



Storage SAN Volumes

- Setup for projects and departments, eg: : /data/cruise, /data/vlf
- Accessible from workstations, bslcenb, bslcenc
- 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

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

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

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

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