POLAR SCIENCE
FOR PLANET EARTH

An Introduction to High Performance Computing 2021

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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.**

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

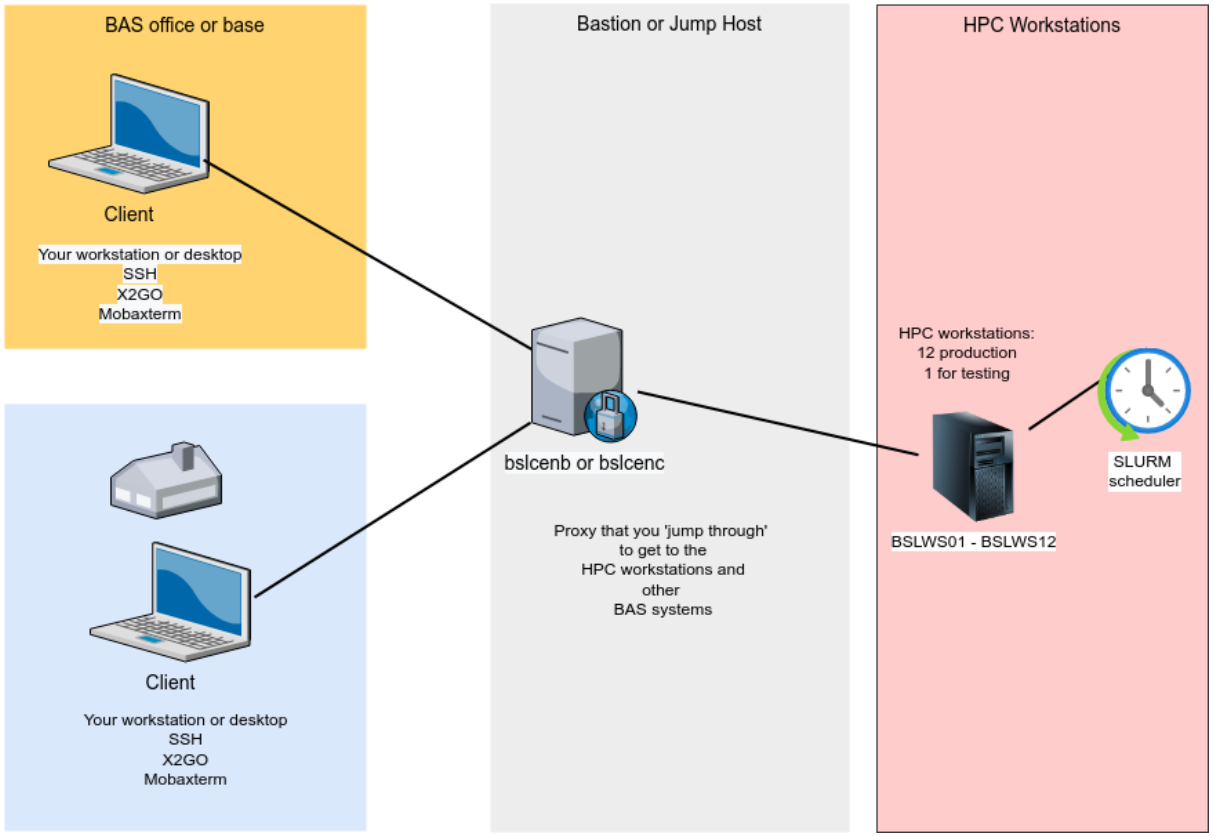
- Gateway or Bastion hosts (bslcenb & bslcenc)
  - Only use for access to BAS or transferring files, donât use for running programs
- Headnodes
  - No access, manages job queues and storage (/data/hpcdata)
- General Use Workstations Private Workstations
- Nodes
- GPU Nodes
  - Currently only available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

Authentication

- Three passwords: 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

Jump or Bastion hosts

To access HPC service you need to pass through our bastion host(s)



SSH

- First connect to jump hosts: bslcenb.nerc-bas.ac.uk or bslcenc.nerc-bas.ac.uk
- Second connect to HPC workstations: bslws01...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

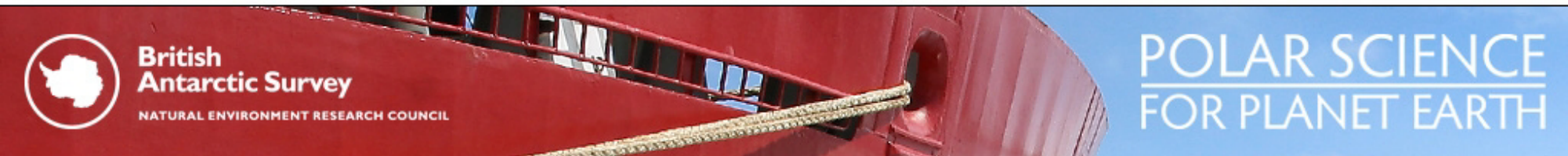
Storage

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.
- Good for transferring multiple files i.e a data set

Data access (SSHFS)

sshfs

- SSHFS client mounts and interacts with directories and files located on a remote systems
- The client uses ssh

Data access (SCP)

Secure Copy Protocol

- Transfer files over ssh
- Good for transferring a small number of files

Part II

User Environment

User Environment

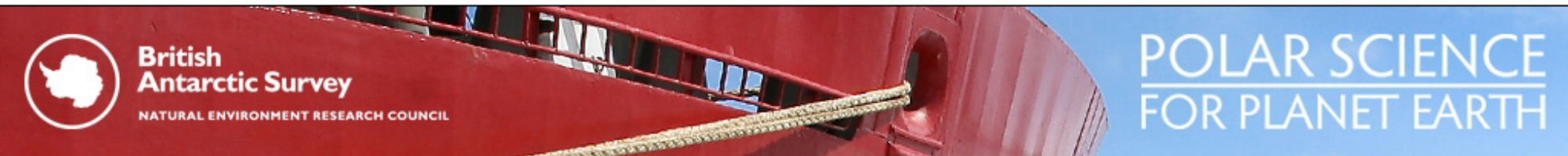
Shell

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

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$_K$*eys*

Demonstration



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

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

The Module System

- Do not work on bslcenb or bslcenc
- 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, $LD_LIBRARY_PATH$ *Loadedmodulesonlyaffecttheterminalyourloadedthemin*

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$_G$*uide*

Demonstration

Jupyter Notebooks

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

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

Containers (cont)

Singularity

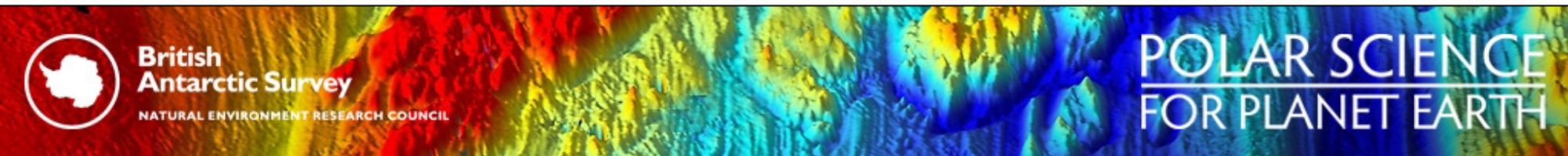
- Designed with HPC usage in mind
- Ready to use on workstations and nodes
- For more information:
  http://ictdocs/wiki/index.php/HPC:Containers
- Demonstration

Part III

SLURM

SLURM

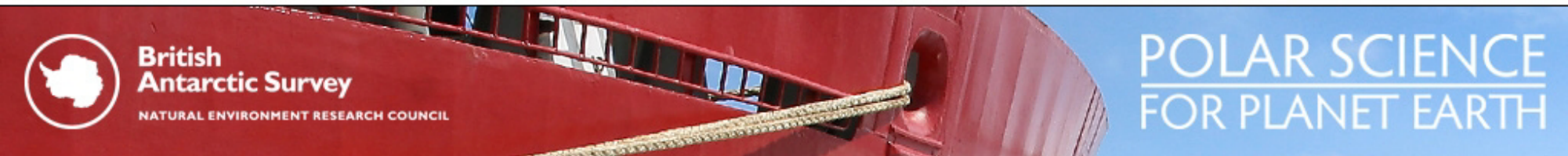
- What is it?
- Simple Linux Utility for Resource Management â our HPC resource manager
- Schedules jobs based on the resources they need



SLURM: Queues

Queues

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



SLURM fair share

Fair Usage

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

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*

SLURM: Job monitoring

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

SLURM: Troubleshooting

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

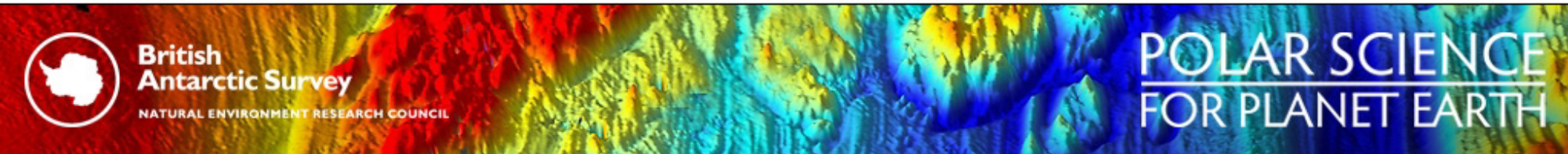
Common mistakes

- 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$_G$*uide*

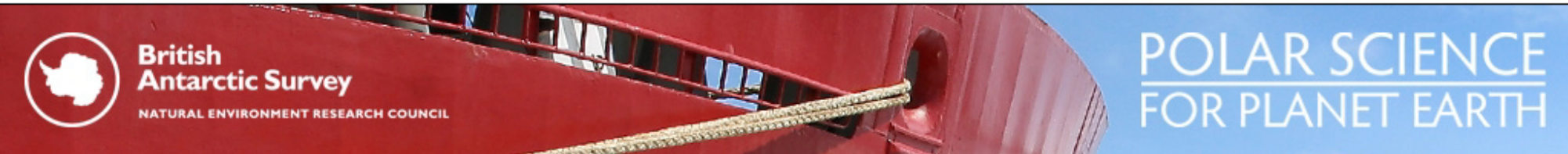
Model Ensembler

- Aimed at solving complex HPC workloads.



Developer Environment

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



Best Practice

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

HELP!

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

Any questions?