POLAR SCIENCE
FOR PLANET EARTH

British Antarctic Survey

HPC Induction 2021

Topics Covered

- Hardware
- Storage
- Access
- Data Transfer
- User Environment
- Software
- Containers
- SLURM
- Model Ensembler
- Best Practice
- HELP!

Hardware

- Gateway or Bastion hosts (bslcenb & bslcenc)
  - Only use for access to BAS or transferring files, don't use for running programs
- Headnodes
  - No access, manages job queues and storage (/data/hpcdata)
- General Use W orkstations & Private W orkstations
- Nodes
- GPU Nodes
  - Currently only available for use BAS AI Lab members
- Development W orkstation and Development Node
  - No access, used for testing by IT

Access

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

SSH

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

Demonstration

Access (continued)

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

Other Options

- Exceed / XMing
- MobaXterm
- Demonstration

Storage

User Area - /users/username

- Small, not intended for sharing data
- Space restricted via quotas

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 (continued)

HPC Storage - /data/hpcdata/ (users, data) & /data/hpcflash

- Accessible from nodes and workstations, bslcenb, bslcenc.
- Usage limited via quotas

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 of fsite, via tapes & disk
- If you need a file restored, contact the service desk

Data Access and T ransfer

Samba

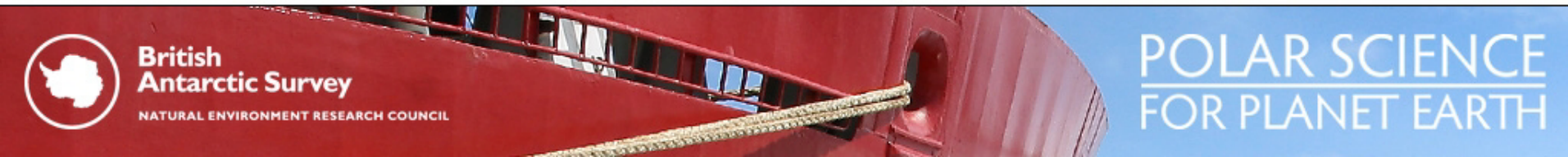
- Allows clients to connect to UNIX storage as if it were a windows network share.
- Allows access to SAN volumes, /users and /data/hpcdata
- No access to /data/hpcflash

FTP

- 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 and T ransfer (continued)

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

User Environment

- Shell
  - Our default shell is tcsh
  - If you prefer something dif ferent such as bash, contact the service desk
- SSH keys
  - Connect to BAS systems without typing passwords
  - ssh-keygen – Always create with a passphrase
  - ssh-agent
  - ./ssh/config
  - More information: http://ictdocs/wiki/index.php/SSH_Keys
  - Demonstration

User Environment

- 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

Software

Operating 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

Modules

- 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. P ATH, LD_LIBRARY_PATH
- Loaded modules only af fect the terminal your loaded them in

Software (continued)

Modules

- Useful module commands:

  module avail module display name/version

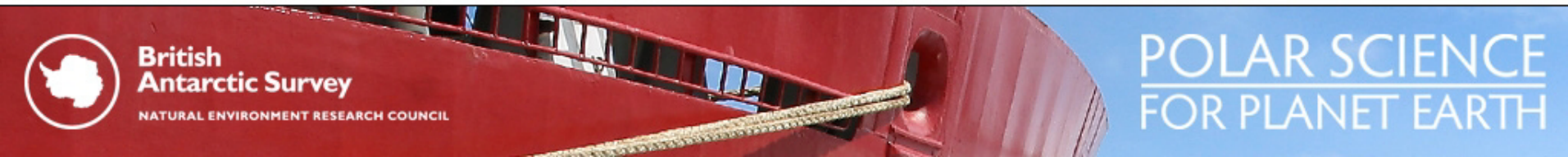
  module load name/version module list

  module unload name/version module purge

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

SLURM

- What is it?
  - Simple Linux Utility for Resource Management – our HPC resource manager
  - Schedules jobs based on the resources they need
- Different queues
  - Short -
  - Medium -
  - Long -
  - GPU -
- 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 – 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 – When you want to run upto a 1000 small jobs
- GPU - To use GPU's you must include the –gres option with the number of GPU's you require:

  #SBATCH –gres=gpu:2

SLURM (continued)

- Job submission scripts – Simple:

- Useful Options
  - Exclusive node: #SBATCH –exclusive
  - Specific node: #SBATCH –nodelist=node022

SLURM (continued)

- Job monitoring

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

SLURM (continued)

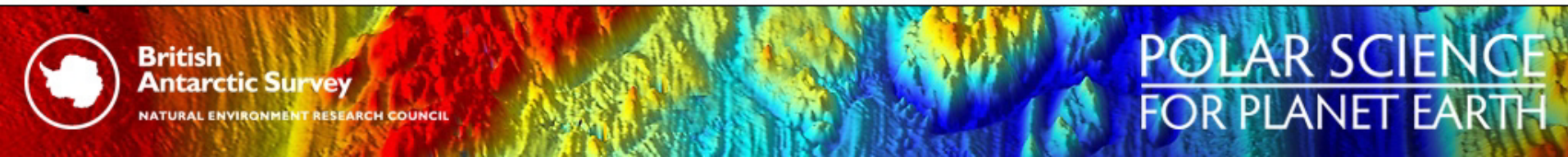
- Troubleshooting failed jobs
  - Set an output file, often has useful information when jobs fail
- Common mistakes
  - Forgetting to load modules
  - Using storage which is not visible to the HPC nodes (use either /data/hpcdata or /data/hpcflash)
  - Avoid using symlinks
  - Did you load any require modules
  - Check your quota
- More information: http://ictdocs/wiki/index.php?title=HPC:User_Guide
- Demonstration

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_Guide

- Service Desk Solutions
- Yammer
- Email List

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Any Questions?

The Following Are Slide Templates

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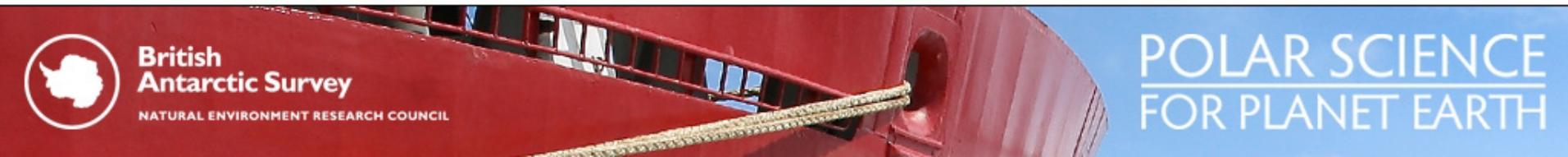
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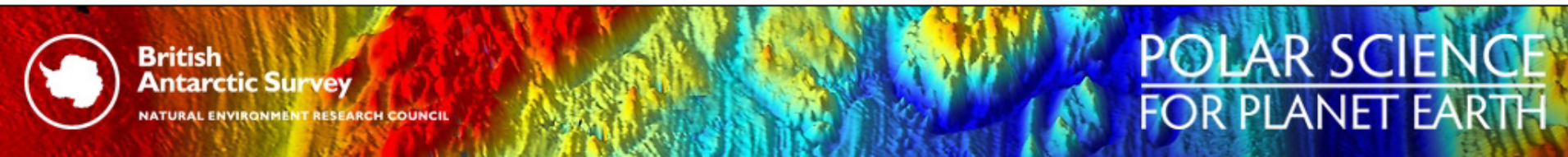
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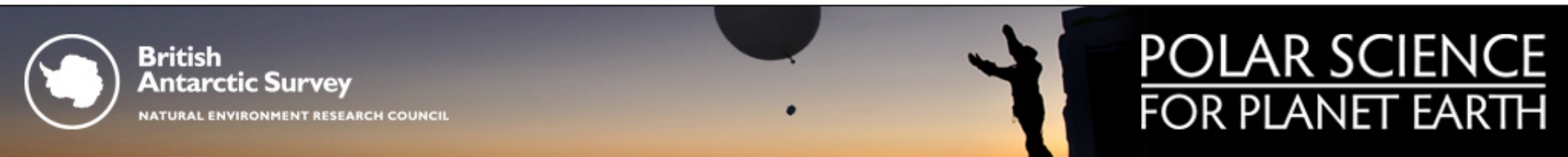
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