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 Workstations & Private Workstations
- Nodes
- GPU Nodes
  - Currently only available for use BAS AILab members
- Development Workstation 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 offsite, via tapes & disk
- If you need a file restored, contact the service desk

Data Access and Transfer

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 Service Desk 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 Service Desk for details

Data Access and Transfer (continued)

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

UserEnvironment

- Shell
  - Our default shell is tcsh
  - If you prefer something different 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

UserEnvironment

- 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. PATH, LD_LIBRARY_PATH
- Loaded modules only affect 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 different compilers
  - Loading clashing modules
- More information: http://ictdocs/wiki/index.php?title=HPC:User_Guide
- Demonstration

JupyterNotebooks

- 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.

DeveloperEnvironment

- 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

POLAR SCIENCE
FOR PLANET EARTH

Any Quest ions?

The Following Are Slide Templates

POLAR SCIENCE
FOR PLANET EARTH

Title

British Antarctic Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL

Title


British
Antarctic Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL
POLAR SCIENCE
FOR PLANET EARTH

Title


British
Antarctic Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL
POLAR SCIENCE
FOR PLANET EARTH

Title

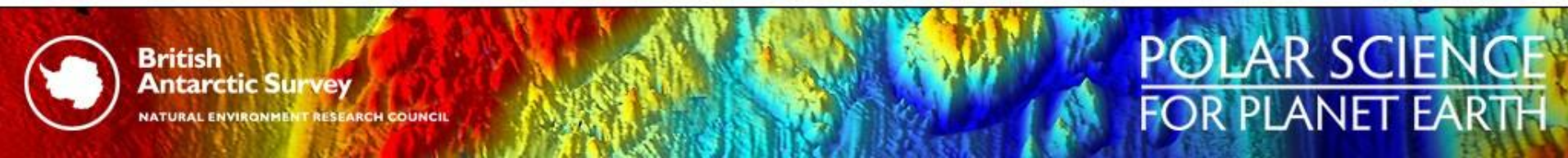

British
Antarctic Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL
POLAR SCIENCE
FOR PLANET EARTH

Title

Title


British
Antarctic Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL
POLAR SCIENCE
FOR PLANET EARTH

Title


British
Antarctic Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL
POLAR SCIENCE
FOR PLANET EARTH

Title


British
Antarctic Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL
POLAR SCIENCE
FOR PLANET EARTH

Title


British
Antarctic Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL
POLAR SCIENCE
FOR PLANET EARTH

Title


British
Antarctic Survey
NATURAL ENVIRONMENT RESEARCH COUNCIL
POLAR SCIENCE
FOR PLANET EARTH