



POLAR SCIENCE FOR PLANET EARTH

British Antarctic Survey

HPC Induction 2021



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Topics Covered

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



Hardware

- Gateway or Bastion hosts (bslce nb & bslce nc)
 - Only use for access to BAS or transferring files, don't use for running programs
- Head nodes
 - 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



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Access

Authentication

- Three passwords – UNIX (NIS), LDAP and Samba,
- UNIX for bslnb /bslnc 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: bslnb.nerc-bas.ac.uk /bslnc.nerc-bas.ac.uk
- Second connect to HPC workstations: bsln01 – bsln12
- 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



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Storage

User Area - /users/user name

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

SAN Volumes

- Set up for projects and departments, eg: : /data/cruise, /data/vlf
- Accessible from workstations, bsce nb, bsce nc
- 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, bsce nb, bsce nc.
- 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



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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

Writable FTP Area

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



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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`



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User Environment

- 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



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



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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 bslnb or bsenc
- 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 e.g. hpc/netcdf/intel/4.4.1.1
- Works by adjusting shell variables e.g. PATH, LD_LIBRARY_PATH
- Loaded modules only affect the terminal you 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:Use_Guide
- Demonstration



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JupyterNotebooks

- 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
- 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
```



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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>`



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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 required modules
 - Check your quota
- More information: http://ictdocs/wiki/index.php?title=HPC:User_Guide
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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 des k: 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?



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The Following Are Slide Templates



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