



An Introduction to High Performance Computing 2021

Paul Sumption
pasump@bas.ac.uk

December 21, 2021



Exercise 1: Login to a BAS HPC Workstation

- ▶ Login to any of the workstations: bslws01...bslws12
- ▶ Configure X2go (it runs on Mac, Linux and Windows)
- ▶ X2go will also allow us to use a graphical desktop in our later exercises



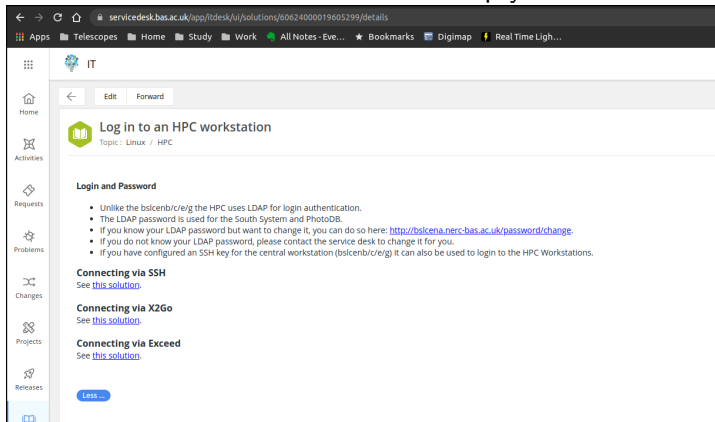
**British
Antarctic Survey**

NATURAL ENVIRONMENT RESEARCH COUNCIL

**POLAR SCIENCE
FOR PLANET EARTH**

Exercise 1: X2go solution

Follow the [service desk solution](#) to setup your client




The screenshot shows a web browser window with the address bar displaying `servicedesk.bas.ac.uk/app/itdesk/ui/solutions/60624000019605299/details`. The browser's address bar also shows several tabs: 'Apps', 'Telescopes', 'Home', 'Study', 'Work', 'All Notes - Eve...', 'Bookmarks', 'Digimap', and 'Real Time Ligh...'. The page content is titled 'IT' and 'Log in to an HPC workstation' with a subtopic of 'Linux / HPC'. It includes a 'Login and Password' section with a bulleted list of instructions: 'Unlike the bsicnrb/c/e/g the HPC uses LDAP for login authentication.', 'The LDAP password is used for the South System and PhotoDB.', 'If you know your LDAP password but want to change it, you can do so here: <http://bsicnrb.cerc-bas.ac.uk/password/change>.', and 'If you do not know your LDAP password, please contact the service desk to change it for you.' It also mentions that an SSH key for the central workstation (bsicnrb/c/e/g) can be used to login to the HPC Workstations. Below this, there are three sections: 'Connecting via SSH' (with a link to 'this solution'), 'Connecting via X2Go' (with a link to 'this solution'), and 'Connecting via Exceed' (with a link to 'this solution'). A 'Less' button is visible at the bottom of the page.

← → ↻ 🏠 `servicedesk.bas.ac.uk/app/itdesk/ui/solutions/60624000019605299/details`

Apps Telescopes Home Study Work All Notes - Eve... Bookmarks Digimap Real Time Ligh...

IT

← Edit Forward

 **Log in to an HPC workstation**
Topic: Linux / HPC

Login and Password

- Unlike the bsicnrb/c/e/g the HPC uses LDAP for login authentication.
- The LDAP password is used for the South System and PhotoDB.
- If you know your LDAP password but want to change it, you can do so here: <http://bsicnrb.cerc-bas.ac.uk/password/change>.
- If you do not know your LDAP password, please contact the service desk to change it for you.
- If you have configured an SSH key for the central workstation (bsicnrb/c/e/g) it can also be used to login to the HPC Workstations.

Connecting via SSH
See [this solution](#).

Connecting via X2Go
See [this solution](#).

Connecting via Exceed
See [this solution](#).

[Less](#)

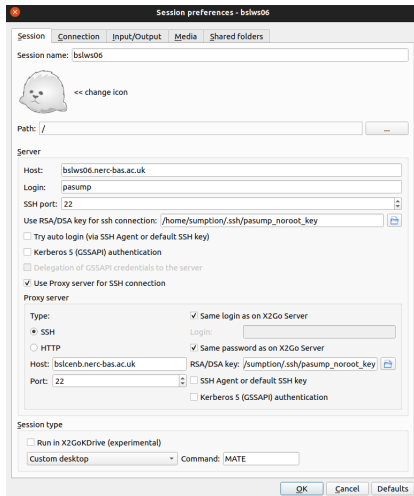


**British
Antarctic Survey**

NATURAL ENVIRONMENT RESEARCH COUNCIL

**POLAR SCIENCE
FOR PLANET EARTH**

Exercise 1: X2go session preferences



The screenshot shows the 'Session preferences - bslws06' window. It has tabs for 'Session', 'Connection', 'Input/Output', 'Media', and 'Shared folders'. The 'Session' tab is active, showing the session name 'bslws06' and a 'change icon' button with a penguin icon. Below this is a 'Path' field set to '/'. The 'Server' section contains fields for 'Host' (bslws06.nerc-bas.ac.uk), 'Login' (pasump), and 'SSH port' (22). It also shows the 'Use RSA/DSA key for ssh connection' path and several checkboxes for authentication methods. The 'Proxy server' section is checked, with 'SSH' selected as the type and fields for 'Host' (bslws06.nerc-bas.ac.uk) and 'Port' (22). The 'Session type' section at the bottom has checkboxes for 'Run in X2GoKDrive (experimental)' and 'Custom desktop', with a 'Command' field set to 'MATE'. At the bottom right are 'OK', 'Cancel', and 'Defaults' buttons.

Session preferences - bslws06

Session Connection Input/Output Media Shared folders

Session name: bslws06

<< change icon

Path: /

Server

Host: bslws06.nerc-bas.ac.uk

Login: pasump

SSH port: 22

Use RSA/DSA key for ssh connection: /home/sumption/.ssh/pasump_noroot_key

☐ Try auto login (via SSH Agent or default SSH key)

☐ Kerberos 5 (GSSAPI) authentication

☐ Delegation of GSSAPI credentials to the server

☒ Use Proxy server for SSH connection

Proxy server

Type: ☒ SSH ☐ HTTP

Same login as on X2Go Server

Login:

Same password as on X2Go Server

Host: bslws06.nerc-bas.ac.uk

Port: 22

RSA/DSA key: /home/sumption/.ssh/pasump_noroot_key

☐ SSH Agent or default SSH key

☐ Kerberos 5 (GSSAPI) authentication

Session type

☐ Run in X2GoKDrive (experimental)

Custom desktop Command: MATE

OK Cancel Defaults

- ▶ Follow the instructions in the solution for your operating system
- ▶ Configure a session preference for a workstation
- ▶ My example uses ssh keys, you can just use passwords



British
Antarctic Survey

NATURAL ENVIRONMENT RESEARCH COUNCIL

POLAR SCIENCE
FOR PLANET EARTH

Exercise 1: X2go session launch



- ▶ Click on a session and launch it
- ▶ You should see a MATE desktop
- ▶ Demonstration
- ▶ Troubleshooting

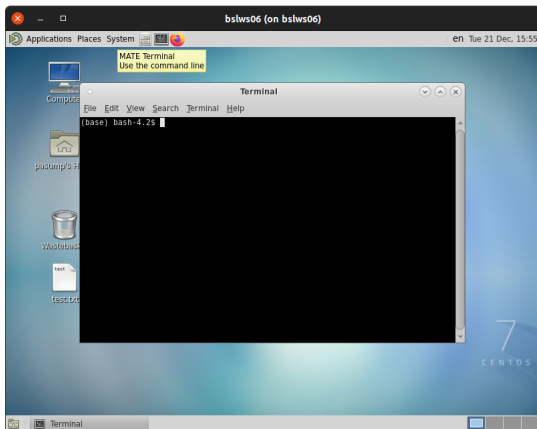


**British
Antarctic Survey**

NATURAL ENVIRONMENT RESEARCH COUNCIL

**POLAR SCIENCE
FOR PLANET EARTH**

Exercise 2: Simple command line operations



- ▶ Click on the terminal icon
- ▶ A terminal window will open
- ▶ We can now interact with our 'shell'



**British
Antarctic Survey**

NATURAL ENVIRONMENT RESEARCH COUNCIL

**POLAR SCIENCE
FOR PLANET EARTH**

Exercise 2: Simple command line operations

- (a) List your current directory (folder) using **ls -al**. Use **df -h** to see the various filesystems, their sizes and their current total usages. You check the hostname of the system using – **hostname**, and **w** to find out who else is using it.
- (b) Examine your personal filesystem quotas with the command **myquota**.

You should see a quota on /users, and a quota on /data/hpcdata as you have two homes.



Exercise 3: File transfer

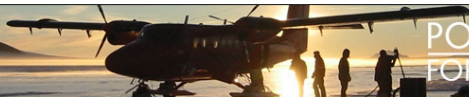
Before attempting exercise 3:

- ▶ http://ictdocs.nerc-bas.ac.uk/wiki/index.php/HPC:User_Guide_Exercises
- ▶ Download the file **exercises.tgz** to your desktop.
- ▶ You will need an sftp client on your laptop to then transfer this file to the cluster.
- ▶ Linux and Mac users - open a terminal, you can use sftp from the command line
- ▶ Windows users - download winsftp



British
Antarctic Survey

NATURAL ENVIRONMENT RESEARCH COUNCIL



POLAR SCIENCE
FOR PLANET EARTH

Exercise 3: File transfer

- Use SFTP to transfer the file **exercises.tgz** to your home directory

Hints: The command is **sftp**. Use the same remote host, username and password as in the previous exercise.

Use **cd rds/hpc-work** to change the target directory, then **put exercises.tgz** to transfer the file from your desktop to the target directory on the Research Computing Service cluster. Use **quit** to close the connection.

Optionally, copy the file over again using **rsync**.



Exercise 3: File transfer (ctd)

- Switch back to the SSH session you created in the previous exercise. Verify that the file is now present by using **ls**.

Hints: Do **ls -al ~/rds/hpc-work/**. Note that you can often reduce typing by pressing **TAB**.

- Unpack the tar archive to create an exercise subdirectory.

Hints: Do **cd ~/rds/hpc-work/** then **tar -zxvf exercises.tgz**.



Exercise 5: Modules and Compilers

- ▶ Go to the **exercises** directory of your cluster account.

Hints: Firstly you may need to review Exercise 1 in order to reconnect to your cluster account. At the remote command prompt, change to the exercises directory (`cd ~/rds/hpc-work/exercises`).

- ▶ Try to compile the **hello.c** program using the default **gcc** compiler (it will fail because there is a deliberate bug).

Hints: `gcc hello.c -o hello`



Exercise 5: Modules and Compilers

- To fix the problem, open the **hello.c** file in an editor (e.g. **gedit**, **nano**, **emacs**).

Hints: Launch gedit in the background by doing **gedit&**. A gedit window should appear. Remove the word **BUG**, save the file and recompile. Do **./hello** to run the program.



British
Antarctic Survey

NATURAL ENVIRONMENT RESEARCH COUNCIL

POLAR SCIENCE
FOR PLANET EARTH

Exercise 5: Modules and Compilers (ctd)

- ▶ The default version of gcc on the RCS HPC clusters is 4.8.5. Compile hello.c again with **gcc 5.4.0**.

Hints: module av, module load, then **gcc hello.c -o hello2**

- ▶ Launch the Matlab GUI. Note this should work from either the SSH command-line or remote desktop sessions.

Hints: **module load matlab** then run: **matlab&**

- ▶ Quit Matlab and launch it again without the graphical desktop interface. This is the way to launch it inside a batch job.

Hints: **matlab -nodisplay -nojvm -nosplash**



Exercise 6: Submitting Jobs (Matlab)

- Submit a job which will run **matlab** on the **file.m** command file (which contains just the Matlab **ver** command).

Hints:

1. Load the matlab module at the place indicated in the file **job_script** in your exercises directory.
2. Set the value of application to **“matlab -nodesktop -nosplash -nojvm”**
3. Set the value of options to **“-r file”**
4. Submit the job with **sbatch job_script**. The jobid is then printed.
5. Watch the job in the queue with **squeue**.
6. After it has disappeared, open the output file **slurm-jobid.out** in your editor. It should contain a list of licensed Matlab features from the ver command.



Exercise 7: Submitting Jobs (serial or threaded application)

- Submit a job which will run a copy of your hello program on 1 cpu.

- Hints:*
1. Edit the script **job_script** in your exercises directory. Set:
#SBATCH --nodes=1
#SBATCH --ntasks=1
application="./hello"
 2. Submit the job with **sbatch job_script**. The jobid is then printed.
 3. Watch the job in the queue with **squeue**.
 4. After it has disappeared, open the output file **slurm-jobid.out** in your editor. There should be exactly one "Hello, World!" message.



Exercise 7: Submitting Jobs (serial or threaded application)

- ▶ Experiment with varying the number of nodes and tasks.
- ▶ Note you will need to launch the application with **srun** to actually use more than 1 cpu.



British
Antarctic Survey

NATURAL ENVIRONMENT RESEARCH COUNCIL



POLAR SCIENCE
FOR PLANET EARTH

Exercise 8: Submitting Jobs (R)

- ▶ R jobs may be serial, threaded, or even MPI parallel depending on the packages used. Submit a job which will run the trivial script **hello.r** program on 1 cpu.

Hints: 1. Edit the script **job_script** in your exercises directory. Set:

```
#SBATCH --nodes=1  
#SBATCH --ntasks=1  
application="Rscript"  
options="hello.r"
```

2. Submit the job with **sbatch job_script**. The jobid is then printed.

- ▶ Repeat this using a different version of R.



Exercise 9: Array Jobs

- ▶ Submit your last job in the form of an array with indices 1-64. Use `-H` with `sbatch` to mark the array as held (so that it won't run immediately).

Hints:

1. Use **`sbatch -H --array=1-64 job_script`**
2. Use **`squeue -u userid`** to see your array job.

Note that `-r` reports each array element individually.



Exercise 9: Array Jobs

- Release array element 1 and allow it to run. Then release the others.

- Hints:*
1. Use **scontrol release**
`${SLURM_ARRAY_JOB_ID}_1`
 2. Use **squeue -u userid** again to watch what happens.
 3. Release the others with
scontrol release
`${SLURM_ARRAY_JOB_ID}`
i.e. use the array id to release the entire array.
 4. When all the jobs complete you should have 64 `slurm-${SLURM_ARRAY_JOB_ID}_N.out` files saying hello from various cpus on possibly multiple nodes.

