Bohrg/Dominion User Documentation

1. What are Bohrg and Dominion?

The Bohrg cluster belongs to the Theoretical Chemistry group in the School of Chemistry[1]. It consists of 115 dual-processor machines. Bohrg was recently (winter 2004/5) re-installed and split into two clusters, Bohrg and Dominion.

The majority of the 115 machines make up *Bohrg*, a "Beowulf" Linux cluster, based on the NPACI Rocks[2]/Redhat[3] distributions. A smaller number make up *Dominion*, a second Beowulf Linux cluster, based on Debian[4].

1.1. Applications

Bohrg

The following applications are installed and available for use on Bohrg:

- Gaussian[5]
- Portland Group[6] Fortran compilers.
- NAG Fortran libraries[7] (for Fortran 77, Mark 20, double-precision).
- Intel Fortran compiler[8], v8.1.

- MPI. . .
- Amber. . .
- Atlas. . .
- GopenMol. . .
- Molden. . .
- Mopac98. . .
- Namd. . .

Dominion

At the time of writing (2005 Apr 18) only Gaussian is available on Dominion, but this will situation will change (improve) in the near future.

[1] http://www.chemistry.manchester.ac.uk/
[2] http://www.rocksclusters.org/
[3] http://www.redhat.com
[4] http://www.debian.org
[5] http://www.gaussian.com
[6] http://www.pgroup.com
[7] http://www.nag.co.uk/
[8] http://www.intel.com/software/products/compilers/flin/

1.2. Hardware

The hardware comprises:

- 115 IBM X330 dual-processor 1133MHz Intel Pentium 3;
- a SCSI array of 9*35Gb disks;

Each node contains:

- 1Gb, 2Gb or 4Gb RAM;
- 1 or 2 20 Gb internal IDE disks.

2. How do I get an account on Bohrg/Dominion?

Accounts on Bohrg and Dominion are available only to staff and students in the Theoretical Chemistry group[9].

To obtain an account, contact Mark Vincent.

You will need to provide Mark with an SSH key. Access to Bohrg and Dominion is by SSH with DSA keys, with passphrase, only — see the sections below on for details.

3. Help!

If you need help relating for Bohrg or Dominion, please:

1. *first read this documentation*;
2. if that does not resolve your problem, speak to Mark Vincent (or perhaps others who have been using the clusters);
3. finally, contact the Specialist Unix Team based at Manchester Computing (details from Mark).

If you have a problem that is not resolved by reading this documentation, please email us so that we can add appropriate information or examples, or improve what is already here.

4. Accessing Bohrg and Dominion — Overview

> *This page is intended to give an overview of accessing the Bohrg and Dominion clusters. More details are given in the sections below (, , . . .); are also given together with some notes on .*

4.1. SSH

Bohrg and Dominion can be accessed only by SSH and related utilities (SCP and SFTP). Furthermore, to increase security SSH on your desktop machine needs to be configured to use a DSA key with a passphrase.

[9] `http://www.chemistry.manchester.ac.uk/research/theoreticalchemistry/`

4.2. Using X-Windows

The X Window System[10] *can* be used to display windows which are "launched" from Bohrg on your local desktop, but such connections must be .

At the time of writing (2005 Apr 14) tunnelling has not been set up on Dominion.

4.3. Gateway Machines

The Bohrg and Dominion clusters are protected by *gateway machines*, called `bohrg1.man.ac.uk` and `bohrg3.man.ac.uk`, respectively. In practice this means that:

- you must login to either `bohrg1` (for Bohrg) or `bohrg3` (for Dominion) and from there login to the (head/submit) node of the cluster itself, rather than accessing the clusters directly;
- setup a SSH DSA key-pair with passphrase before you can use either cluster.

4.4. Head/Submit Nodes

Behind the gateway machines, each cluster consists of a "head" or "submit" node and a number of "compute" nodes. Jobs are submitted to the batch-queueing system (SGE) from the head/submit nodes; jobs run on the compute nodes. (There is no reason for users to login to the compute nodes.)

Bohrg

The head node for this cluster is called `storage`. (This node doubles as the machine on which the SCSI disk array resides.)

Dominion

The head node for this cluster is called `dominion1`.

5. Gateways: bohrg1 and bohrg3

5.1. Network Topology

Both the Bohrg and Dominion clusters exist on private networks for security reasons. In order to access either cluster, users must first login to a gateway machine: for the Bohrg cluster, this is `bohrg1.man.ac.uk`, and for the Dominion cluster, this is `bohrg3.man.ac.uk`.

Each gateway machine has two network connections — one facing the public Internet, the other facing the private network on which the cluster sits.

5.2. Home Directories

Users' home directories on `bohrg1` and `bohrg3` are local and unconnected to home directories on the Bohrg and Dominion clusters.

[10] `http://www.x.org/X11.html`

5.3. Firewalling

Both gateway machines have default-deny firewalls configured, i.e., most connections, inward and outward, whether originating from the outside world, the Bohrg or Dominion cluster, or from the machines themselves, are blocked.

Almost the only permitted connection is into `bohrg1`/`bohrg3` via SSH.

5.4. Restricted User Environment on `bohrg3`

Users will find that once authenticated to `bohrg3` their environment is *severely* restricted: almost the only action available to users is to `ssh` into the Dominion cluster. This has been done for security reasons.

5.5. Copying Files to/from Bohrg and Dominion (NAT/Forwarding)

Occasionally it is desirable to launch a connection from, say, the Bohrg cluster, to the outside world. For example, you may want to copy (via SCP) a file to your desktop machine. This is handled by *network address translation* and connection *forwarding* on the gateway; it is completely transparent to users and *makes it possible to* `scp` *a file from the head/submit nodes to the outside world in one step, rather than by first copying it to the gateway* — for details, see the FAQ.

6. OpenSSH Access to The Gateways — Keys and Passphrase

> *This page describes how to set up a DSA key/passphrase to securely connect from your desktop machine (client) to* `bohrg1` *and/or* `bohrg3` *using OpenSSH (with SSH protocol 2).*

To be absolutely clear, we are using:

- OpenSSH[11], *not* the version from <XLNK="">SSH Communications Security[12], on both client and server;
- we use DSA keys, not RSA keys, and
- SSH Protocol 2 (not 1 or 1.5).

(If you wish to use an SSH client from SSH Comms on your desktop machine, you are on your own!)

[11] `http://www.openssh.org`
[12] `http://www.openssh.org`

6.1. Prerequisites

1. Ensure you have an up-to-date version of OpenSSH installed on your desktop machine. Furthermore, ensure that no other implementation of SSH, e.g., that from SSH Communications Security (`www.ssh.com`) is around to confuse the issue.

2. Ensure that on your desktop machine, within your home directory, a sub-directory called `.ssh` exists and that the permissions are correct, e.g.,

   ```
   drwx------   2 simonh users     136 2005-01-05 12:17 .ssh
   ```

   i.e., the directory is private to the owner.

6.2. Generating, Installing and Testing the Key

1. First we make the key. On your local/client desktop machine type

```
ssh-keygen -t dsa
```

You will be prompted for the name of a file in which to keep the key (the default is fine). You will also be prompted for a passphrase — *don't use a blank or easily-guessed passphrase.* You will see something like this:

```
prompt> ssh-keygen -t dsa
Generating public/private dsa key pair.
Enter file in which to save the key (/home/mc/.ssh/id_dsa):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in /home/mc/.ssh/id_dsa.
Your public key has been saved in /home/mc/.ssh/id_dsa.pub.
The key fingerprint is:
e0:..........................................:xy user@clienthost
prompt>
```

Two files are created: `~/.ssh/id_dsa` and `~/.ssh/id_dsa.pub`. The first is your private key; the second is your public key.

2. Copy your public key to your `.ssh` directory on `bohrg1` and/or `bohrg3` — ask Mark Vincent to do this.

3. Test that the key-pair is working — make use of your SSH client's verbose mode to do this:

```
ssh -v bohrg1.man.ac.uk -l simonh -v

OpenSSH_3.8p1, SSH protocols 1.5/2.0, OpenSSL 0.9.7d 17 Mar 2004
debug1: Reading configuration data /etc/ssh/ssh_config
debug1: Applying options for *
debug2: ssh_connect: needpriv 0
debug1: Connecting to bohrg1.man.ac.uk [130.88.200.111] port 22.
debug1: Connection established.
.
.
debug1: identity file /home/simonh/.ssh/id_dsa type 2
debug1: Remote protocol version 2.0, remote software version OpenSSH_3.4p1 Debian 1:3.4p1-
1.woody.3
.
.
debug1: Host 'bohrg1.man.ac.uk' is known and matches the RSA host key.
debug1: Found key in /home/simonh/.ssh/known_hosts:1
.
.
debug1: Authentications that can continue: publickey,password,keyboard-interactive
debug1: Next authentication method: publickey
```

Notice the available methods of authentication and their order: `publickey`, `password` and `keyboard-interactive`. The first is our key-with-passphrase-based method; the others are password-only-based methods (used above to copy `id_dsa.pub` to the remote machine).

```
.
.
debug1: Offering public key: /home/simonh/.ssh/id_dsa
.
.
Enter passphrase for key '/home/simonh/.ssh/id_dsa':
```

Enter your passphrase and hit `return`, and you will be authenticated and logged in as usual.

7. PuTTY Access to The Gateways — Keys and Passphrase

8. Submit Nodes: storage and dominion1

8.1. Network Topology

To access the Bohrg or Dominion Cluster users should login to the appropriate head or submit node, `storage` for Bohrg and `dominion1` for Dominion, via the appropriate .

8.2. Home Directories

On login to *both* `storage` and `dominion1` users will find themselves in their home-directory mounted from the SCSI array attached to `storage` as

```
/home/bohrg/<username>
```

(`/home/dominion/<username>` is *not* used on Dominion). This home-directory is shared across the two clusters, i.e., users' will see the same files on both machines.

8.3. Scratch Space

On login to *both* `storage` and `dominion1` users will be able to access their scratch space mounted from the SCSI array attached to `storage` as

```
/scratch/bohrg/<username>
```

(`/scratch/dominion/<username>` is *not* used on Dominion). This scratch space is shared across the two machines.

8.4. Submitting and Monitoring Jobs: SGE

Users must never run jobs on `storage` *or* `dominion1`*; all jobs should be submitted to the* . SGE can also be used to monitor the progress of jobs.

8.5. Access to the Outside World

For information on access *from* the Bohrg and Dominion clusters *to* the outside world, especially copying files, see the FAQ.

8.6. Access to Compute Nodes

There is usually no reason for users to access the compute nodes on either cluster (except via the SGE). (When code and scripts are being developed, such access can be justified.)

At the time of writing (2005 April 18) users can login to the compute nodes on the Bohrg cluster, but cannot login to the compute nodes on the Dominion cluster. In the near future user access to the compute nodes on Bohrg will be blocked.

9. Example Login Sessions

9.1. Accessing the Bohrg Cluster

Following is a simple example session in which I begin at my desktop machine as user `simonh`, `ssh` into `bohrg1` and from there into `storage`, the head/submit node for the Bohrg cluster.

First, login to `bohrg1` — note that a passphrase for a key is prompted for:

```
simonh@mctalby: $ ssh mpciish2@bohrg1.man.ac.uk
Enter passphrase for key '/home/simonh/.ssh/id_dsa':

****************************************************************************
    This is the Bohrg gateway, bohrg1.man.ac.uk (aka bohrg.man.ac.uk).
    Any questions or problems to Mark Vincent in the first instance.
****************************************************************************

Last login: Fri Apr 15 13:27:41 2005 from mctalby.mc.man.ac.uk

mpciish2@bohrg1: $ ls -al
total 20
drwxr-xr-x    3 mpciish2 users        4096 Apr  6 13:56 .
drwxr-xr-x    3 root     root         4096 Feb 27 17:43 ..
-rw-------    1 mpciish2 users          52 Apr  6 13:55 .Xauthority
-rw-------    1 mpciish2 users         313 Apr 15 13:32 .bash_history
drwx------    2 mpciish2 users        4096 Apr  6 13:55 .ssh
```

If you are not prompted for a *passphrase for a key*, something is not working correctly and you will not be able to login. Notice the directory called `.ssh` and the permissions on that directory (it is private).

Next, login to `storage`:

```
mpciish2@bohrg1: $ ssh storage
mpciish2@storage's password:
Rocks 3.1.0 (Matterhorn)

Profile built 17:25 09-Oct-2004
Kickstarted 17:25 09-Oct-2004

-bash-2.05b$ ls -F
src/               trash/                compat-libstdc++-7.3-2.96.118.i386.rpm
pgi_master_license  RaidMan-7.00.i386.rpm
-bash-2.05b$ ls -F
```

Notice that this is *not* the same home directory as that on `bohrg1`.

From here, storage, I can use SGE to submit and monitor jobs:

```
-bash-2.05b$ qstat

 job-ID  prior name       user         state submit/start at     queue      master  ja-task-
ID
------------------------------------------------------------------------------------------------

   1075     0 a4aEZRRCa  mbdtsmv      r     04/05/2005 10:05:18 compute-0- MASTER
            0 a4aEZRRCa  mbdtsmv      r     04/05/2005 10:05:18 compute-0- SLAVE
   1211     0 r_h2o_3
   .
   .
   .
```

9.2. Accessing the Dominion Cluster

Following is a simple example session in which I begin at my desktop machine as user simonh, ssh into bohrg3 and from there into dominion1, the head/submit node for the Dominion cluster.

First, login to bohrg3 — note that a passphrase for a key is prompted for:

```
simonh@mctalby:$ ssh mpciish2@bohrg3.man.ac.uk
Enter passphrase for key '/home/simonh/.ssh/id_dsa':
Last login: Wed Apr  6 13:40:07 2005 from mctalby.mc.man.ac.uk
-bash-2.05b$ ls
-bash: ls: command not found
-bash-2.05b$ telnet
-bash: telnet: command not found
-bash-2.05b$ pwd
/home/mpciish2
```

Notice that the environment is severely restricted — neither ls nor telnet are available. (pwd is built in to the shell.)

Next, login to `dominion1`:

```
-bash-2.05b$ ssh dominion1
Password:
Linux dominion1 2.4.27 #2 SMP Mon Mar 7 17:42:23 GMT 2005 i686 GNU/Linux

The programs included with the Debian GNU/Linux system are free software;
the exact distribution terms for each program are described in the
individual files in /usr/share/doc/*/copyright.

Debian GNU/Linux comes with ABSOLUTELY NO WARRANTY, to the extent
permitted by applicable law.

Last login: Tue Mar 22 09:44:37 2005 from 10.2.62.250

mpciish2@dominion1:$ ls -F
src/                trash/              compat-libstdc++-7.3-2.96.118.i386.rpm
pgi_master_license  RaidMan-7.00.i386.rpm
mpciish2@dominion1:$
```

Notice that the files visible are the same as those on `storage` (above) as the home-directories are shared between the two clusters.

10. Tunnelling X-Windows through SSH

Traditionally X-Windows applications can be started on a remote server and displayed on your local desktop by means of commands like `xhost +bohrg.man.ac.uk` *(on your local machine) and* `export DISPLAY=mymachine.ch.man.ac.uk` *(on the remote server). This method is insecure and is blocked on Bohrg and Dominion. Instead, tunnel your display through SSH as described below.*

10.1. Tunnelling X-Windows Applications on the Bohrg Cluster

Following is a simple example in which I begin at my desktop machine as user `simonh`, `ssh` into `bohrg1` and then `storage`, and from there start a graphical, X-aware client which displays in a new window on my local desktop.

First, login to `bohrg1`, note the `-X` option which enables X-Windows forwarding (*not* `-x`, which *dis*ables forwarding):

```
simonh@mctalby:$ ssh -X bohrg1.man.ac.uk -l mpciish2
Enter passphrase for key '/home/simonh/.ssh/id_dsa':
Warning: No xauth data; using fake authentication data for X11 forwarding.

***************************************************************************

    This is the Bohrg gateway, bohrg1.man.ac.uk (aka bohrg.man.ac.uk).

    Any questions or problems to Mark Vincent in the first instance.

***************************************************************************
Last login: Fri Apr 15 13:32:12 2005 from mctalby.mc.man.ac.uk
mpciish2@bohrg1:$
```

Note the line `Warning: No xauth data; using fake authentication data for X11 forwarding.` Now confirm that your SSH client and the SSH server on `bohrg1` are in agreement that X11 traffic should be forwarded:

```
mpciish2@bohrg1:$ echo $DISPLAY
localhost:19.0
mpciish2@bohrg1:$
```

If, instead of `localhost:19.0` or similar (the number will vary), you see nothing, or something like `desktop.ch.man.ac.uk:0`, then chances are that tunnelling is not set up. (In the former case `bohrg1` is not set up to attempt to display any X-Windows application on your desktop; in the latter case it is attempting to bypass the SSH connection and make a new connection in the "old fashioned" way — this will fail.)

Next, login to `storage`:

```
mpciish2@bohrg1:$ ssh -X storage
mpciish2@storage's password:
Rocks 3.1.0 (Matterhorn)
Profile built 17:25 09-Oct-2004

Kickstarted 17:25 09-Oct-2004
-bash-2.05b$
```

Notice that again I have specified the `-X` (uppercase) option. Again it is worth confirming that tunnelling is set before starting a graphical client in the background:

```
-bash-2.05b$ echo $DISPLAY
localhost:19.0
-bash-2.05b$ xclock &
[1] 12390
-bash-2.05b$
```

The clock should appear on your local desktop, perhaps after a few seconds.

10.2. Tunnelling X-Windows Applications on the Dominion Cluster

At the time of writing (2005 Apr 18) X-Windows applications cannot be tunnelled through SSH on the Dominion cluster. This situation will change in the near future.

11. File System Overview

This page is intended to offer an overview of the filesystems on the Bohrg and Dominion clusters which are of interest to users. More information is available on the pages below (, and).

11.1. Hardware/Disks

The “core” storage on Bohrg and Dominion is based around an array of SCSI disks which is physically attached to `storage`, the head/submit node for Bohrg.

In addition, each node contains 1 or 2 internal disks.

11.2. Central Filesystems

The following filesystems live on the central SCSI disk and are *automounted* on `dominion1` (head/submit node for Dominion) and on all the compute nodes (on both clusters):

```
/home/bohrg/<username>
/scratch/bohrg/<username>
/software/bohrg/<application>
```

These are, respectively, users’ home directories, users’ central scratch space and the applications available, such as Gaussian and the PGI compilers.

11.3. Local Filesystems

On each node, spare disk space has been allocated as scratch space. Currently this is accessible as

```
/tmp               # Bohrg compute nodes
/local_scratch     # Dominion compute nodes
```

A naming convention which will apply across all nodes will hopefully be worked out soon!

11.4. Automounted Filesystems

All filesystems which live on the central SCSI disk are *automounted* to make them available to users. This means that they are mounted on demand and if they are not used for a specified time they are unmounted.

11.5. Automounted Filesystems — A Warning

The automounter can cause confusion. Here is an example:

```
bohrg> cd /software
bohrg> ls -a
    .  ..
bohrg> cd bohrg                    # or cd ./bohrg
bohrg> ls -a
    amber  gaussian...
```

Automounted directories are mounted on demand — listing the *parent* directory does *not* count as demand!

12. Home Directories

12.1. Home Directories on the Bohrg and Dominion Clusters

Each user of the Bohrg and Dominion clusters has a home-directory which lives on the central disk array — this directory is shared between the two clusters (i.e., users will see the same files on `dominion1` as on `storage`).

Users will find themselves in their home-directory on login. These directories are *automounted* and accessible as

```
/home/bohrg/<username>
```

on `storage`, `dominion1` and both sets of compute nodes.

12.2. Home Directories on the Gateway Machines

Home-directories on `bohrg1` and `bohrg3` are completely independent of those on the clusters; they live on the internal disks of the gateway machines.

This said, for backup purposes, and so as to help file transfer between Bohrg (and Dominion), and the outside world, home-directories from `storage` are accessible as `/home/bohrg/<username>` on `bohrg1` (not on `bohrg3`) — this access is *read-only* for security-related reasons.

12.3. Quotas

There are currently no home-directory quotas in operation. If space becomes short quotas will be introduced.

12.4. Backups

Home-directories are backed up. In the event of a disk-crash (or accidental file deletion) files stored in home-directories will be restored. Backups are taken on most days, so that restored directories (or files) should normally be at most a few hours out of date.

13. Scratch Space

13.1. Central Scratch Space

A total of 67Gb is currently available for central scratch space. This space is shared amongst all users. Each user has a directory within the central scratch space allocated to them. This directory is automounted as

```
/scratch/bohrg/<username>
```

on both `storage` and `dominion1` (the head/submit nodes), and on all compute nodes.

13.2. Scratch Space Local to Compute Nodes

All compute nodes have scratch space available to users on a local/internal disk. I/O to local scratch space should be faster than to central scratch space.

The amount of local scratch space available varies from node to node, but a minimum of 8.2Gb should be available on all nodes:

Dominion

On Dominion 8.2Gb of scratch space is available on each node. This is currently mounted on `/scratch_local`

Bohrg

On Bohrg, some machines have one internal disk while others have two, so that the amount of local scratch space available varies considerably. Roughly speaking, nodes making up the "Big Mem queue" (more accurately, *parallel environment*) have 19Gb, while the other nodes have 14Gb.

13.3. Rules of Usage

...

13.4. Links from Home Directories to Central Scratch Space

...

13.5. Tidy-Up Scripts

On some machines hosted by Manchester Computing scratch space is regularly "tidied up", e.g., files created more that a month ago are automatically deleted. At present (2005 Apr 19) there is no such automated deletion. Should scratch space become short this automation might be introduced.

13.6. Quotas

There are currently no scratch space quotas in operation. If space becomes short quotas will be introduced.

13.7. Backups

Scratch space is *not* backed up. Do not store any files in scratch space which you need to keep or cannot easily reproduce (e.g., from a re-run of a job).

14. Software: `/software`

15. Running Gaussian on Storage and Dominion1

1. First you will need to set up your environment such that it knows about the batch system.
   a. For Storage and Dominion1 edit your `.profile` (`ksh` and `bash` users) and add to your path the location of `qsub` (needed by `toq`):
      ```
      export PATH=$PATH:/usr/local/sge_5.3p6/bin/glinux
      ```
   b. Also, in your .profile put the location of SGE via
      ```
      export SGE_ROOT=/usr/local/sge_5.3p6
      ```
   c. To make these changes take effect type
      ```
      . .profile
      ```

4. You will need to get a copy of the `RunGauss` script:
   a. For **Storage** copy the `RunGauss` script from `/usr/local/bin` to you own file space (your own `bin` directory would be an ideal place for it!). Use this version in your own filestore for all calculations.
   b. For **Dominion1** copy the `RunGaussDom` from `/usr/local/bin` to your own filestore (i.e. `~/bin/RunGaussDom`). Use this version to run jobs.
   c. Use the `-g03` option of `RunGauss` (i.e. `~/bin/RunGauss -g03 -i job.com -o job.out` or `RunGaussDom -g03 -i input.com -o output.out`).

4. Use the **toq** script to submit jobs:
   a. An example of the use of the **toq** script is
      ```
      /usr/local/bin/toq -nodes 1 -procs 2 -q any_std -lt 96:0:0 -r jobname runscript
      ```

Needless to say `jobname` is your name for the job and `runscript` is your script that has the `Rungauss` (or `RunGaussDom`) command in it. Note `runscript` should be executable (i.e. to make executable do: `chmod a+x runscript`). `any_std` is the queue the job will run in (it has a time limit of 96:0:0 hours, hence `-lt 96:0:0`). Note that most jobs will only need to use this queue, however, there is a `bigmem` queue on Storage which has a time limit of 120:0:0 hours and a larger memory size (hence the name).

16. Amber

???

17. User Environment

Should all just work, but just in case here is what to check:

```
-- user environment :
    -- echo $PATH, echo $MANPATH
    -- PATH=.....:/software.....
    -- MANPATH=.......

-- /etc/profile, /etc/bashrc, /.profile, /.bashrc
```

Shell:

```
-- ksh and bash;
-- chsh...
```

18. Software/Applications

```
-- pgi compilers
    -- PGI_ROOT=/software/pgi-524
    -- LM_LICENSE_FILE="7496@psico.ch.man.ac.uk"

-- gaussian

--
```

19. The Batch/Queue System — SGE

Environment should be set up for you vi `/etc/profile`, but if there is a problem please check:

```
-- export SGE_ROOT=/usr/local/sge_5.3p6
-- PATH includes...
-- MANPATH includes...
```

Using:

```
-- qstat
--
```

20. Why do we need to use SSH keys, they make life difficult!

Yes, unfortunately the use of SSH keys (with passphrases) can be confusing. SSH is far more complex than Telnet — there at least 4 authentication methods, some of which involve keys, and there are different types of keys too.

(To access `bohrg1` and `bohrg3`, follow these notes[13], the section on *Key/Passphrase Authentication* in particular. N.B. Use DSA keys to access these machines, nor RSA keys.)

[13] `../_ssh`

At the time of writing (2005/April/05) accounts on HPC machines connected to the Internet are increasingly being compromised, globally. Frequently this is done by first compromising the desktop machine from which a user logs in to the HPC machine; key-grabbing software is often installed on such compromised desktops. The use of keys with passphrases means that an HPC account cannot be compromised by this method.

21. How do I copy files to/from Bohrg/Dominion?

21.1. General

There is no FTP access to or from Bohrg/Dominion. Neither can the "r"-commands be used, e.g., `rcp`. The only way to copy files to or from Bohrg/Dominion is to use `scp` or `sftp`.

21.2. Possible Connections

Recipes for copying files to and from Bohrg and Dominion are given below. By way of background information the following information can be noted:

To/from `bohrg1/3`

- SSH/SCP/SFTP connections from the outside world *to* `bohrg1` and `bohrg3` are permitted (DSA key and passphrase required), but
- SSH/SCP/SFTP connections *from* `bohrg1` and `bohrg3` to the outside world are blocked for security-related reasons.

To/from `storage/dominion1`

- *Direct* SSH/SCP/SFTP connections from `storage` and `dominion1` to the outside world are possible (such connections travel through `bohrg1` or `bohrg3` transparently thanks to the wonders of network address translation).
- It is not possible to make any direct connection from the outside world to `storage` or `dominion1` for security-related reasons.

21.3. Additional Info

The following information is also pertinent:

- home directories from `storage` are accessible *read-only* on `bohrg1`, as `/home/bohrg/<username>`.

21.4. Recipes

To download to your desktop machine from `storage` or `dominion1`

From you desktop machine, `scp` or `sftp` files from `/home/bohrg/<username>` on `bohrg1`.

Notes:

1. that this accessibility is read-only, so you cannot upload files to `storage` by this means;
2. it is not possible to download files from `bohrg3` in this manner.

To upload from your desktop to `storage` or `dominion1`

1. From your desktop machine, `scp` or `sftp` files to `/home/<username>` on `bohrg1` or `bohrg3`.
2. From `bohrg1` or `bohrg3`, `scp` or `sftp` files to `storage` or `dominion1`.

Unfortunately, an upload requires two steps (though see below).

For those few running an SSH/SCP/SFTP service/daemon on their desktop machine, it is possible to reduce the previous recipe to a single step. N.B. *Running such a service on your desktop machine has significant security implications, so do not do this unless you are confident that you fully understand patching, firewalls and intrusion detection.*

To download to, or upload from, your desktop machine to/from `storage` or `dominion1`, if your desktop machine is running an SSH daemon

Login to `storage` or `dominion1` in the usual way. From there, `scp` or `sftp` directly to your desktop machine. For example:

```
storage> scp fred@desktop.ch.man.ac.uk:myfile myfilehere
```

or,

```
storage> scp myfile fred@desktop.ch.man.ac.uk:myfilethere
```

22. How do I use X-Windows to view graphical applications?

bohrg1/storage

```
 1. desktop> ssh -X bohrg1.man.ac.uk -l <username>

        -- "-X" not always required, depends on config on your desktop machine,
           but will do no harm;

        -- NOT "-x";

 2. bohrg1> ssh storage

 3. storage>xterm &

     -- do not "export DISPLAY=..." or "setenv DISPLAY ..."
     -- do not su at any stage
```

bohrg3/dominion1

```
 -- not at the moment, to come...
```

23. How do I access the machines from home?

The machines are firewalled and are accessible from Chemistry (130.88.80.*, 130.88.83.*, 130.88.12.*) and from The University VPN[14], only. So if you wish to login from home, you must use the VPN.

About this page:

Produced from the SGML: /home/mc/public_html/_bohrg/_reml_grp/bohrg_dominion_user_doc.reml

On: 12/12/2005 at 13:43:19

Options: reml2 -l nolong -o tex -p single

[14] http://www.mcc.ac.uk/vpn/