

CHPC Lengau – First-Time Access Guide

Overview

To improve security, the CHPC Lengau cluster now uses **SSH key authentication** instead of passwords. This guide walks you through the complete process-from logging into the CHPC User Portal to successfully accessing the Lengau cluster.

Before You Begin

Please ensure you have the following:

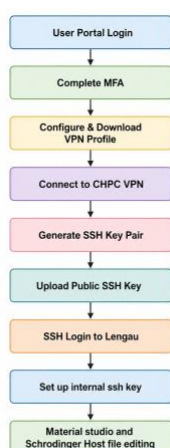
- Your CHPC username and password.
- Access to your registered email account (for Multi-Factor Authentication).
- A stable internet connection.
- A VPN client installed on your computer

Useful Resources

Resources	Link
CHPC User Portal	https://users.chpc.ac.za/
VPN Configuration Guide	https://wiki.chpc.ac.za/guide:vpn
VPN Client Downloads	wireguard.com/install
SSH Key Documentation	https://wiki.chpc.ac.za/guide:sshkeys
CHPC User Documentation	https://wiki.chpc.ac.za/start - getting startedthe quickstart guide

Workflow Overview

Follow the steps below **in order**.



Step 1 – Log in to the CHPC User Portal

1. Open the **CHPC User Portal** (<https://users.chpc.ac.za/>)
2. Enter your CHPC username and password.
3. Click **Login**.

Step 2 – Complete Multi-Factor Authentication (MFA)

1. A **6-digit verification code** will be sent to your registered email address.
2. Enter the code on the verification page.
3. Click **Verify**.

Step 3 – Configure and Download Your VPN Profile

After successful login:

1. Open the **VPN Configuration** page (<https://users.chpc.ac.za/vpn/>)
2. Generate your VPN profile.
3. Download the generated **.ovpn** file.

Step 4 – Connect to the CHPC VPN (<https://wiki.chpc.ac.za/guide:vpn>)

1. Open your VPN client.
2. Import the downloaded **.ovpn** profile.
3. Connect to the CHPC VPN.

Confirm that the VPN connection is successful before continuing.

Important: You must be connected to the CHPC VPN before attempting to access the Lengau cluster.

Step 5 – Generate an SSH Key Pair (<https://wiki.chpc.ac.za/guide:sshkeys>)

If you already have an SSH key pair, you may skip this step.

Otherwise, generate one on your local computer.

Step 6 – Upload Your Public Key

1. Return to the CHPC User Portal.
2. Open **SSH Key Management**.
3. Paste the copied public key.
4. Click **Save**.

Step 7 – Connect to Lengau

Open your terminal (or SSH client) and connect:

```
ssh <username>@lengau.chpc.ac.za
```

If your SSH key is registered correctly, you will be logged in without being asked for your CHPC password.

Note: “Couldn’t resolve host name: Host name unknown” when trying to login indicate that you’re not connected to the VPN.

What to do when you get such error. Perform VPN Debug checklist:
[https://wiki.chpc.ac.za/quick:login?s\[\]=%2Achecklist%2A#checklist](https://wiki.chpc.ac.za/quick:login?s[]=%2Achecklist%2A#checklist)

Step 8- Setting up Internal ssh key

1. Navigate to your SSH directory:

```
cd ~/.ssh
```

2. List the contents to verify your SSH keys:

```
ls -l
```

3. If you see the cluster-generated keys (`id_hpc_mpi` and `id_hpc_mpi.pub`), use those. Otherwise, if you have generated an ECDSA key, use `id_ecdsa.pub`.

4. Check whether your public key is already in `authorized_keys`:

```
cat authorized_keys
```

5. If using the cluster-generated key:

```
cat id_hpc_mpi.pub
```

or, if using an ECDSA key:

```
cat id_ecdsa.pub
```

6. If the public key is **not** already present in `authorized_keys`, append it:

For the HPC key:

```
cat id_hpc_mpi.pub >> authorized_keys
```

or for an ECDSA key:

```
cat id_ecdsa.pub >> authorized_keys
```

Important: Always use `>>` and **not** `>`. The `>>` operator appends the public key to the existing `authorized_keys` file, whereas `>` overwrites the file and may remove other authorised keys.

7. Confirm that the key has been added:

```
cat authorized_keys
```

Step 9- Host file editing for Schrödinger and Material studio

You will need to **edit your “hosts.” file** (with no extension). The edit is done by copying this *hosts* file to one of your own dirs such as Documents, edit there, and then copy file back (in the etc\ dir you can't easily edit directly). Do the copy as Administrator (and using Admin elsewhere may help too).

Please make sure you add the following line in the
C:\Windows\System32\drivers\etc\hosts file

10.128.15.123 mslogin.chpc.ac.za mslogin

Remove any other line such as.

196.24.44.123 mslogin.chpc.ac.za mslogin