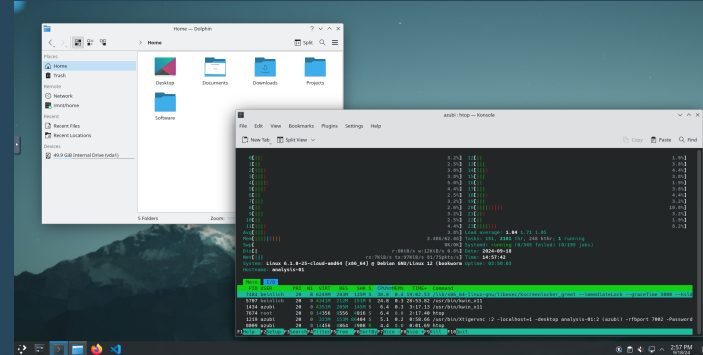




ANALYSIS-0X & GPU-0X

FIRST STEPS ON THE VIRTUAL DESKTOP SERVERS

Simeon Beinlich
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PP&B Computer Support Group
Fritz-Haber-Institut der Max-Planck-Gesellschaft





REGISTRATION

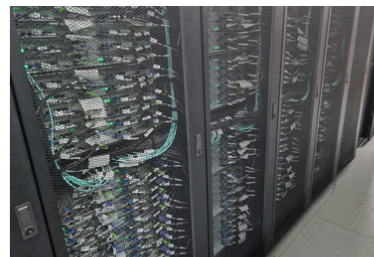
In order to use the one of the analysis servers, please register here:
<https://root.compute.fhi.mpg.de>.

Enter your:

- Full name
- Your FHI email address
- Choose a user/project name
(ideally the FHI username)
- Your use case

Specify **that you need a virtual desktop session**

Shortly after you will receive a confirmation email
with your login credentials.



FHI Compute Manager

Welcome to the FHI Compute Manager!

Create User / Project Account

Your Full Name

Fhi User

Your E-Mail

fhiusername@fhi.mpg.de

Your username / projectname

fhiusername

Use-case

Access Jupyterhub and a virtual
desktop session for python
postprocessing.

Create Account



REGISTRATION | LOGIN CREDENTIALS

Shortly after you will receive a confirmation email with your login credentials.

Dear User,

You can now log in to the compute servers, e.g. jupyterhub-01, analysis-01, gpu-01, storage-01, etc. instances with your new compute credentials:

- **username:** *yourusername*
- **initial password:** *yourpassword*

Virtual desktop session:

- **hostname:** analysis-02
- **link:** [https://analysis-02.compute.fhi.mpg.de:6080/\[...\]](https://analysis-02.compute.fhi.mpg.de:6080/[...])
- **username:** *yourusername*
- **token** (*ID of your desktop*): 28g0358-g54226-25h62-235z-vq45g564

Please keep this information safe, and change your initial password!

Dear User frosch,

You can now log in to the compute servers, e.g. jupyterhub-01, analysis-01, gpu-01, storage-01, etc. instances with your new compute credentials:

- **username:** frosch
- **initial password:** qgbqetqtb

Please change your password immediately as described here:

- Changing your password: <https://gitlab.fhi.mpg.de/fhi-hpc/jupyterhub-compute/-/wikis/Access>

You can access the following virtual desktop sessions:

Virtual desktop session:

- hostname: analysis-02
- **link:** [https://analysis-02.compute.fhi.mpg.de:6080/\[...\]](https://analysis-02.compute.fhi.mpg.de:6080/[...])
- username: frosch
- **token:** qgvqet-rvq4-2r1f3-qf1t-34g34qqg

Documentation:

Please have a look at the ppb wiki page: <https://ppbwiki.fhi.mpg.de/Main/HPC> and the documentation of the compute services:

General:

- Changing your password: <https://gitlab.fhi.mpg.de/fhi-hpc/jupyterhub-compute/-/wikis/Access>

Jupyterhub:

- Wiki: <https://gitlab.fhi.mpg.de/fhi-hpc/jupyterhub-compute/-/wikis/HOME>
- Usage: <https://gitlab.fhi.mpg.de/fhi-hpc/jupyterhub-compute/-/wikis/Usage>



CHANGING YOUR PASSWORD

Visit: root.compute.fhi.mpg.de.

Click on **Change Password**.

Enter your

- **username:** *yourusername*
- **initial password:** *yourpassword*

Set a

- *new password*

Please use at least 8 characters containing letters, numbers, and symbols.

FHI Compute Manager

Welcome to the FHI Compute Manager!



Change Your Password

Your username / projectname

Old Password:

New Password

Confirm New Password

Change Password



RESTART YOUR VNC SESSIONS

After changing your password, you will be asked, whether you **want to restart all your VNC sessions to inherit the password.**

Confirm this by clicking **Start / restart all VNC Sessions**.

FHI Compute Manager

Welcome to the FHI Compute Manager!



Password changed successfully. It might take up to a minute until the password has been synchronized to all services.

Please as well use the new password when connecting to the storage server(s) and remember to restart all your VNC sessions to inherit the password change.

Start / restart all VNC Sessions

Back to main menu



RESTART YOUR VNC SESSIONS

After changing your password, you will be asked, whether you **want to restart all your VNC sessions to inherit the password.**

Confirm this by clicking **Start / restart all VNC Sessions**.

Enter again your

- **username:** *yourusername*

and the

- **new password**

and click **(Re)start**.

FHI Compute Manager

Welcome to the FHI Compute Manager!



Password changed successfully. It might take up to a minute until the password has been synchronized to all services.

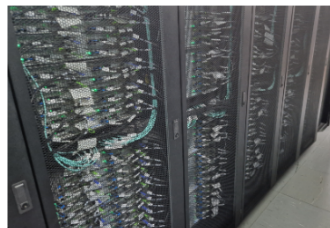
Please as well use the new password when connecting to the storage server(s) and remember to restart all your VNC sessions to inherit the password change.

Start / restart all VNC Sessions

Back to main menu

FHI Compute Manager

Welcome to the FHI Compute Manager!



Start / restart all VNC Sessions

Your username / projectname

Password

(Re)start



RESTART YOUR VNC SESSIONS

After changing your password, you will be asked, whether you **want to restart all your VNC sessions to inherit the password.**

Confirm this by clicking **Start / restart all VNC Sessions**.

Enter again your

- **username:** *yourusername*

and the

- **new password**

and click **(Re)start**.

**Restart your VNC Sessions whenever you experience problems,
or if your session was shut down.**

It is equivalent to logging out and login in again.

FHI Compute Manager

Welcome to the FHI Compute Manager!



Password changed successfully. It might take up to a minute until the password has been synchronized to all services.

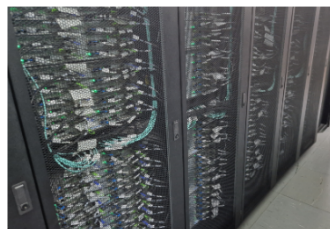
Please as well use the new password when connecting to the storage server(s) and remember to restart all your VNC sessions to inherit the password change.

Start / restart all VNC Sessions

Back to main menu

FHI Compute Manager

Welcome to the FHI Compute Manager!



Start / restart all VNC Sessions

Your username / projectname

Password

(Re)start



DESKTOP ACCESS VIA BROWSER

You can now access your desktop session!

Open a browser (we recommend Chrome) and enter **the link you received upon registration:**

- **link:** [https://analysis-02.compute.fhi.mpg.de:6080/\[...\]](https://analysis-02.compute.fhi.mpg.de:6080/[...])

Click **Connect**.





DESKTOP ACCESS VIA BROWSER

You can now access your desktop session!

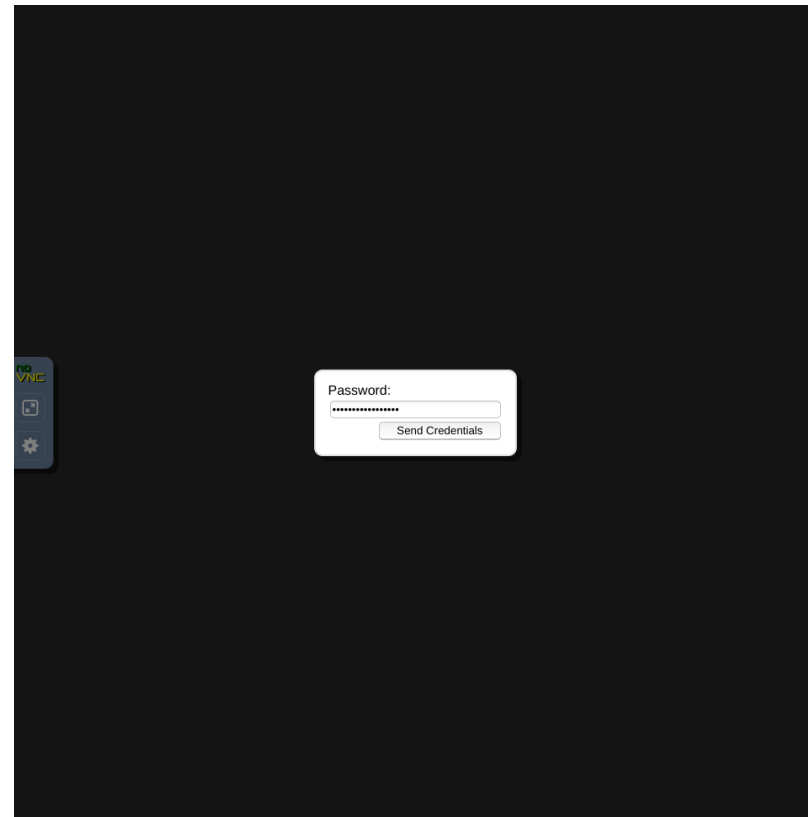
Open a browser (we recommend Chrome) and enter **the link you received upon registration**:

- **link:** [https://analysis-02.compute.fhi.mpg.de:6080/\[...\]](https://analysis-02.compute.fhi.mpg.de:6080/[...])

Click **Connect**.

Enter your password: *new password*

Click **Send Credentials**





DESKTOP ACCESS VIA BROWSER

You can now access your desktop session!

Open a browser (we recommend Chrome) and enter **the link you received upon registration**:

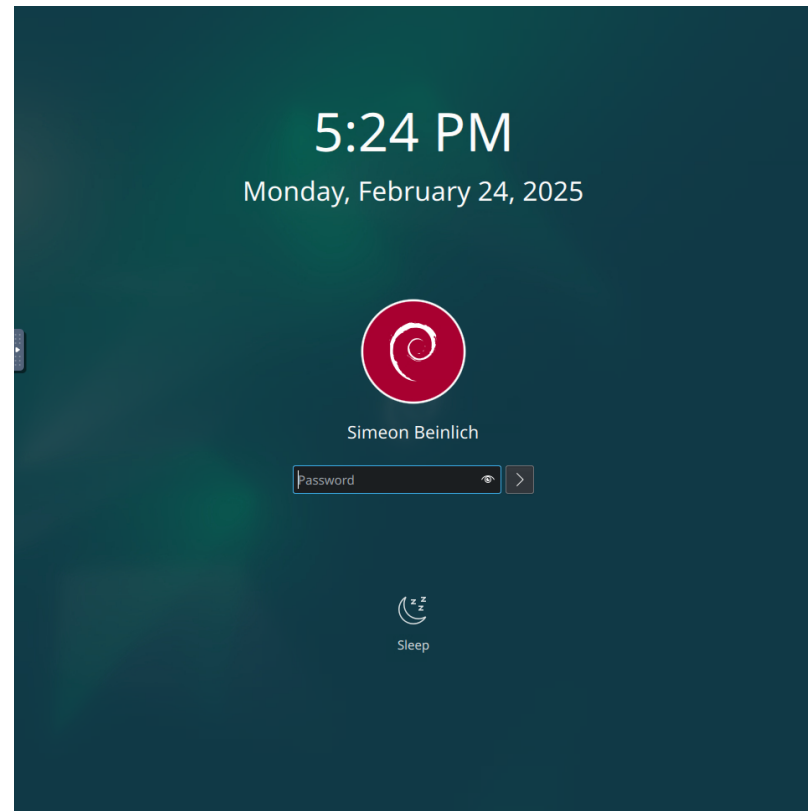
- **link:** [https://analysis-02.compute.fhi.mpg.de:6080/\[...\]](https://analysis-02.compute.fhi.mpg.de:6080/[...])

Click **Connect**.

Enter your password: *new password*

Click **Send Credentials**

You might encounter a lock screen as shown on the right, just **enter your password again**.





DESKTOP ACCESS VIA BROWSER

You can now access your desktop session!

Open a browser (we recommend Chrome) and enter **the link you received upon registration**:

- **link:** [https://analysis-02.compute.fhi.mpg.de:6080/\[...\]](https://analysis-02.compute.fhi.mpg.de:6080/[...])

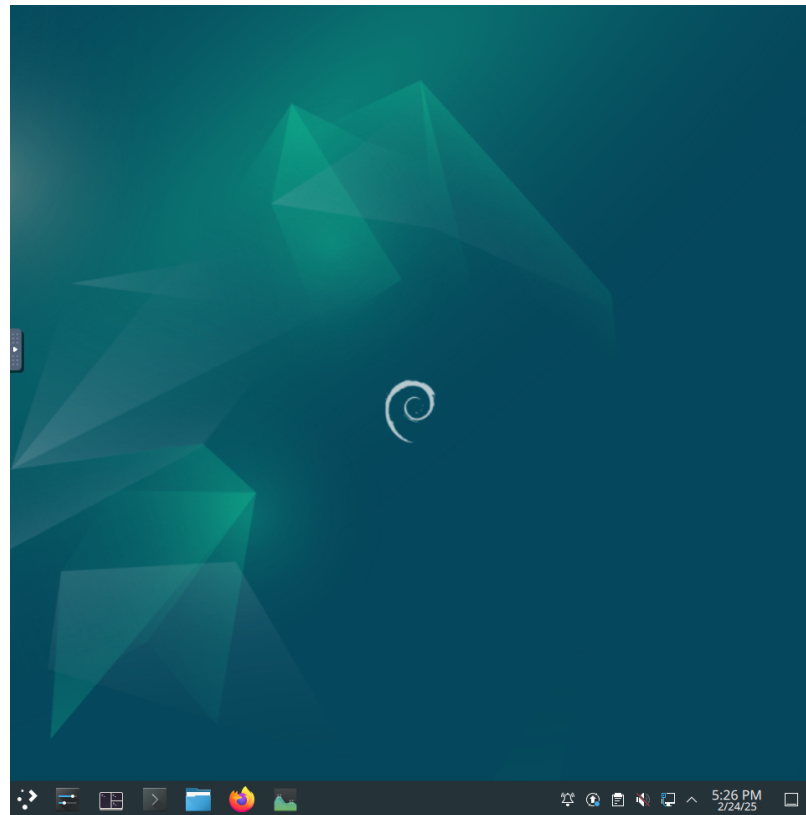
Click **Connect**.

Enter your password: *new password*

Click **Send Credentials**

You might encounter a lock screen as shown on the right, just **enter your password again**.

Welcome to your desktop environment!





DESKTOP ACCESS VIA BROWSER

You can now access your desktop session!

Open a browser (we recommend Chrome) and enter **the link you received upon registration**:

- **link:** [https://analysis-02.compute.fhi.mpg.de:6080/\[...\]](https://analysis-02.compute.fhi.mpg.de:6080/[...])

Click **Connect**.

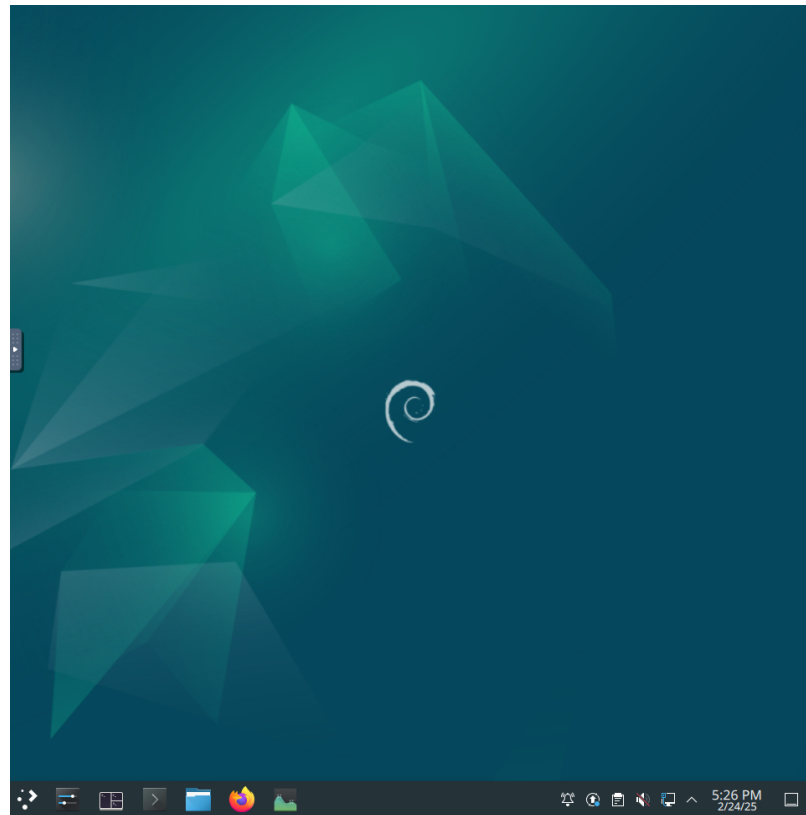
Enter your password: *new password*

Click **Send Credentials**

You might encounter a lock screen as shown on the right, just **enter your password again**.

Welcome to your desktop environment!

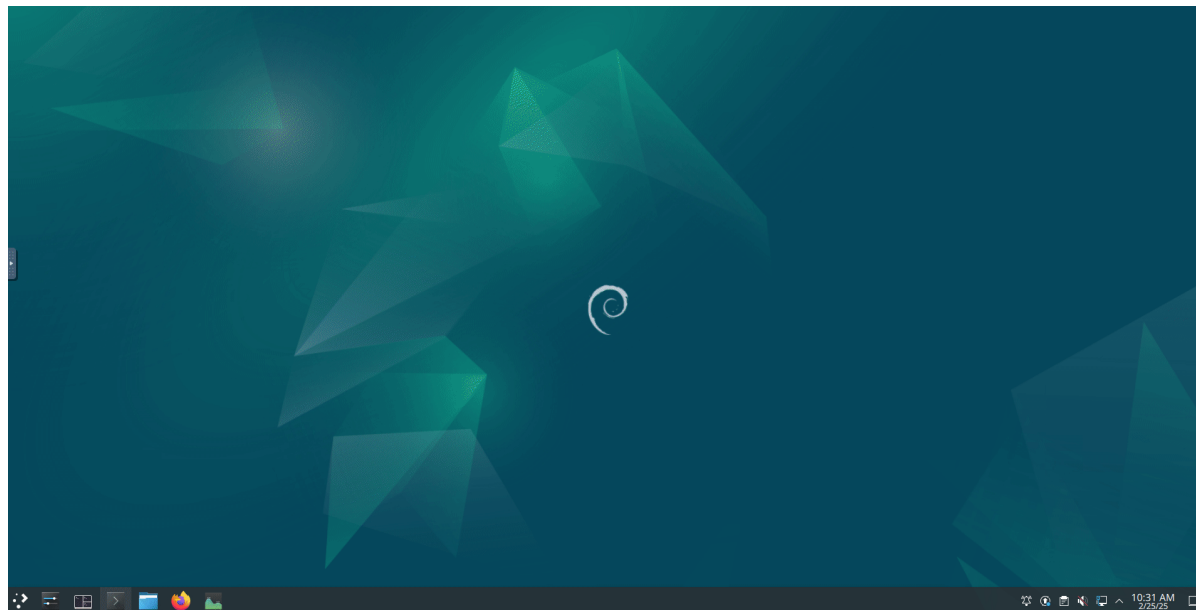
If any dialogs pop up in the beginning, just close them.





USING THE DESKTOP ENVIRONMENT

You can now use the desktop environment as if it was your laptop!

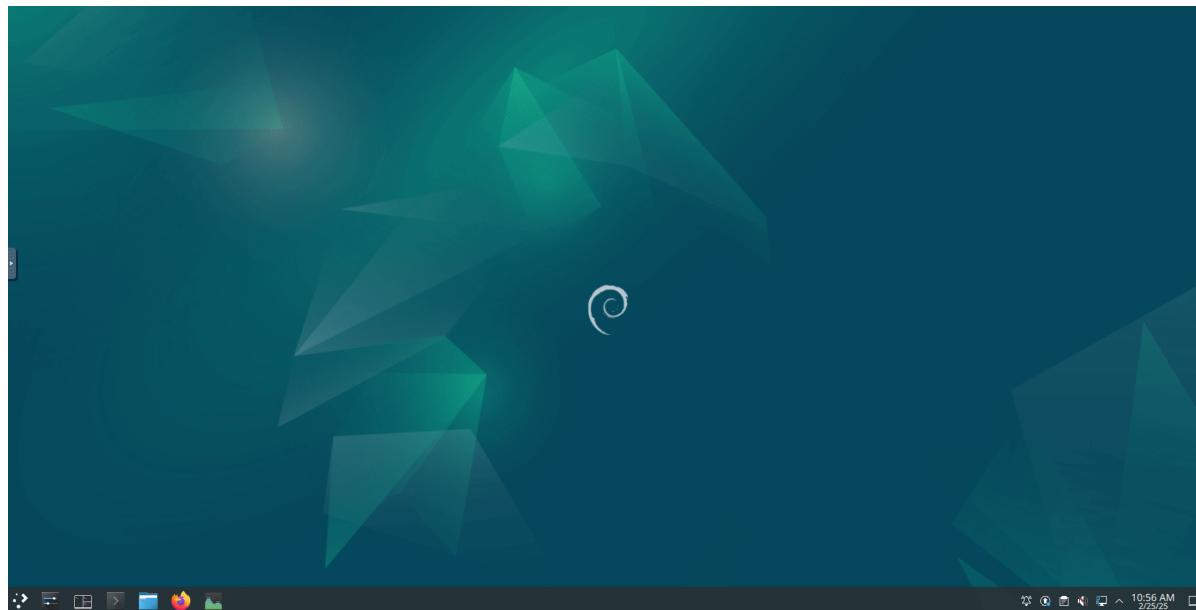


Gaussian + GView



USING THE DESKTOP ENVIRONMENT

You can now use the desktop environment as if it was your laptop!

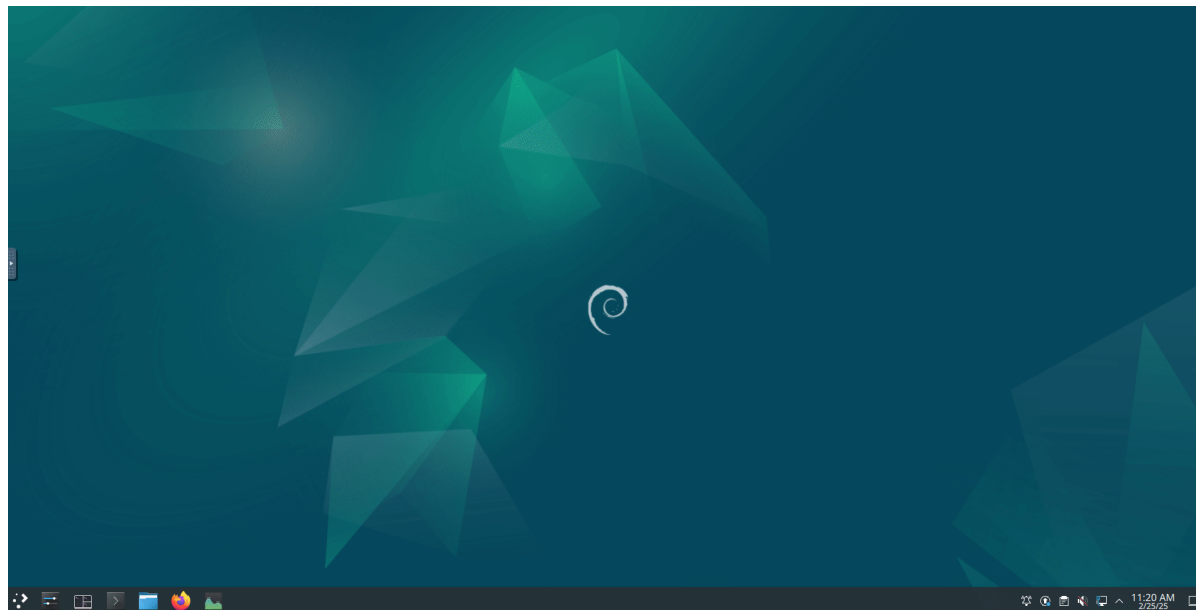


Python: conda environment + ipython



USING THE DESKTOP ENVIRONMENT

You can now use the desktop environment as if it was your laptop!

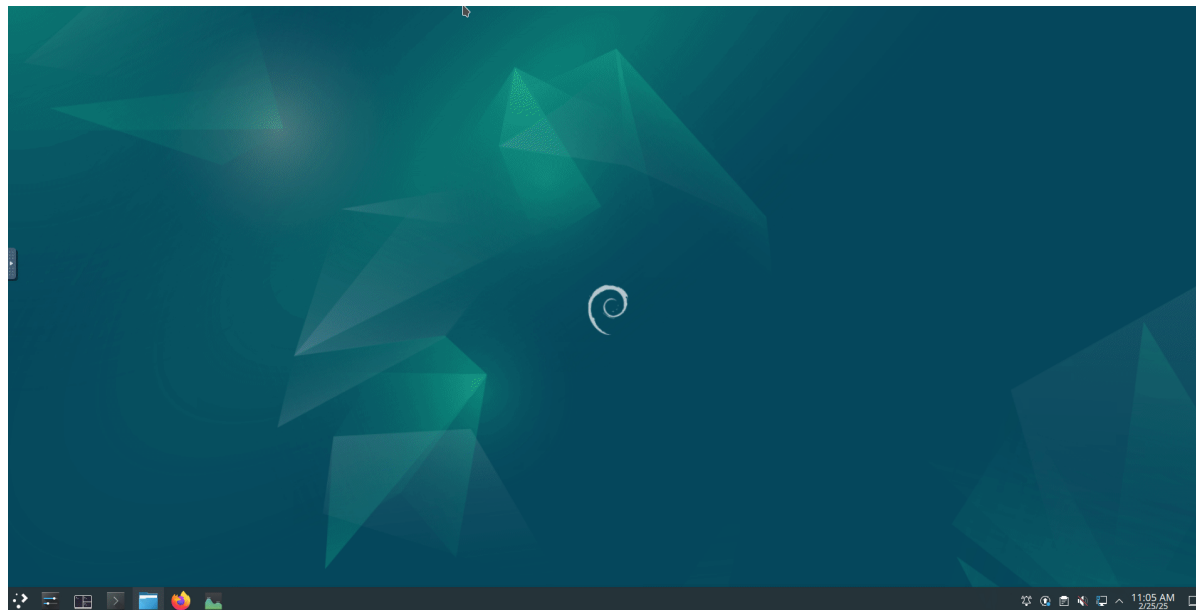


Python: Jupyter Notebooks



USING THE DESKTOP ENVIRONMENT

You can now use the desktop environment as if it was your laptop!



VScode: any programming, e.g. python multiprocessing notebooks



AVAILABLE SOFTWARE

SCIENTIFIC

- Abinit + abipy
- Avogadro
- Crest
- CP2K
- Dirac
- Gaussian 16
- GaussView 6
- HDFview
- Molpro
- Orca
- Vesta
- ...

PROGRAMMING

- Python
- Matlab
- C, C++, Fortran
- ...

IDE

- VScode
- Spyder
- VIM
- ...

COMPILERS

- GNU compilers
 - gfortran
 - gcc
 - g++
- Openmpi
- Nvidia HPC SDK & CUDA
- ...

Any Linux Software can be installed - and maybe some Windows software.



CUSTOM SOFTWARE

Any Linux Software can be installed - and maybe some Windows software.

You need **privileged permissions**?

You need **help setting up** your software or you **can't find it**?

You don't know **where to start**?

Please get in touch!



TERMINAL ACCESS VIA SSH

You have terminal / SSH access to all compute servers!

Be sure to connect to the machine you need (analysis-01, -02, -03, ...)!

LINUX, MACOS, WINDOWS POWERSHELL

Open a terminal on your laptop and connect via ssh. You can then run any command.

```
1 ~$ ssh frosch@analysis-01.compute.fhi.mpg.de
2
3 frosch@analysis-01.compute.fhi.mpg.de's password:
4 Linux analysis-01 6.1.0-31-cloud-amd64 #1 SMP PREEMPT_DYNAMIC Debian 6.1.128-1...
5 Last login: Tue Oct 15 15:55:33 2024 from 172.18.0.102
6
7 (base) frosch@analysis-01:~$ ll
8
9 total 8
10 lrwxrwxrwx 1 root   root   9 Oct 22 14:44 data -> /mnt/data
11 drwx----- 1 frosch ac    20 Oct 24 15:41 Desktop
12 drwxr-xr-x 1 frosch ac     0 Dec 19 09:05 Documents
13 drwxr-xr-x 1 frosch ac     0 Dec 19 09:05 Downloads
14 lrwxrwxrwx 1 root   root  10 Oct 22 14:44 local -> /mnt/local
15 drwxr-xr-x 1 frosch ac     0 Dec 19 09:05 Music
16 [...]
17 (base) frosch@analysis-01:~$
```



TERMINAL ACCESS VIA SSH

You have terminal / SSH access to all compute servers!

Be sure to connect to the machine you need (analysis-01, -02, -03, ...)!

LINUX, MACOS, WINDOWS POWERSHELL

Open a terminal on your laptop and connect via ssh. You can then run any command.

```
1 ~$ ssh frosch@analysis-01.compute.fhi.mpg.de
2
3 frosch@analysis-01.compute.fhi.mpg.de's password:
4 Linux analysis-01 6.1.0-31-cloud-amd64 #1 SMP PREEMPT_DYNAMIC Debian 6.1.128-1...
5 Last login: Tue Oct 15 15:55:33 2024 from 172.18.0.102
6
7 (base) frosch@analysis-01:~$ ll
8
9 total 8
10 lrwxrwxrwx 1 root    root    9 Oct 22 14:44 data -> /mnt/data
11 drwx----- 1 frosch  ac      20 Oct 24 15:41 Desktop
12 drwxr-xr-x 1 frosch  ac       0 Dec 19 09:05 Documents
13 drwxr-xr-x 1 frosch  ac       0 Dec 19 09:05 Downloads
14 lrwxrwxrwx 1 root    root   10 Oct 22 14:44 local -> /mnt/local
15 drwxr-xr-x 1 frosch  ac       0 Dec 19 09:05 Music
16 [...]
17 (base) frosch@analysis-01:~$
```



TERMINAL ACCESS VIA SSH

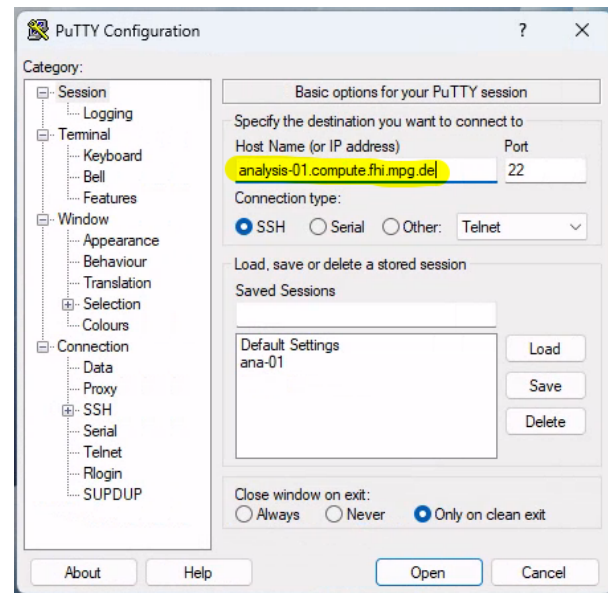
You have terminal / SSH access to all compute servers!

Be sure to connect to the machine you need (analysis-01, -02, -03, ...)!

WINDOWS PUTTY

Open Putty

- Enter the address `analysis-01.compute.fhi.mpg.de`
- Click **Open**
(You can as well **Save** this session!)





TERMINAL ACCESS VIA SSH

You have terminal / SSH access to all compute servers!

Be sure to connect to the machine you need (analysis-01, -02, -03, ...)!

WINDOWS PUTTY

Open Putty

- Enter the address `analysis-01.compute.fhi.mpg.de`
- Click `Open`
(You can as well `Save` this session!)
- Enter your *username*, press `Enter`
- Enter your *password* (invisible), press `Enter`.

```
1 login as: frosch
2 frosch@analysis-01.compute.fhi.mpg.de's password:
3 Linux analysis-01 6.1.0-31-cloud-amd64 #1 SMP ...
4 Last login: Tue Feb 25 11:55:56 2025 from 141.14.136.106
5 (base) frosch@analysis-01:~$ ls
6 data      Documents  local      Pictures   Templates
7 Desktop   Downloads  Music      Public     Videos
8 (base) frosch@analysis-01:~$ cd Downloads/
9 (base) frosch@analysis-01:~/Downloads$ ls
10 some-file.txt
11 (base) frosch@analysis-01:~/Downloads$ cat some-file.txt
12 Some content
13 (base) frosch@analysis-01:~/Downloads$ cd ..
14 (base) frosch@analysis-01:~$
```



TERMINAL ACCESS VIA SSH

You have terminal / SSH access to all compute servers!

Be sure to connect to the machine you need (analysis-01, -02, -03, ...)!

WINDOWS PUTTY

Open Putty

- Enter the address `analysis-01.compute.fhi.mpg.de`
- Click `Open`
(You can as well `Save` this session!)
- Enter your **username**, press `Enter`
- Enter your **password** (invisible), press `Enter`.

Enter any commands, e.g.:

- list the content of this folder: `ls`
- go into a folder: `cd Downloads`
- show the content of a file: `cat some-file.txt`
- go one folder up: `cd ..`

```
1 login as: frosch
2 frosch@analysis-01.compute.fhi.mpg.de's password:
3 Linux analysis-01 6.1.0-31-cloud-amd64 #1 SMP ...
4 Last login: Tue Feb 25 11:55:56 2025 from 141.14.136.106
5 (base) frosch@analysis-01:~$ ls
6 data      Documents  local      Pictures   Templates
7 Desktop   Downloads  Music      Public     Videos
8 (base) frosch@analysis-01:~$ cd Downloads/
9 (base) frosch@analysis-01:~/Downloads$ ls
10 some-file.txt
11 (base) frosch@analysis-01:~/Downloads$ cat some-file.txt
12 Some content
13 (base) frosch@analysis-01:~/Downloads$ cd ..
14 (base) frosch@analysis-01:~$
```



TERMINAL ACCESS VIA SSH

You have terminal / SSH access to all compute servers!

Be sure to connect to the machine you need (analysis-01, -02, -03, ...)!

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Open Putty

- Enter the address `analysis-01.compute.fhi.mpg.de`
- Click `Open`
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- Enter your *username*, press `Enter`
- Enter your *password* (invisible), press `Enter`.

Enter any commands, e.g.:

- list the content of this folder: `ls`
- go into a folder: `cd Downloads`
- show the content of a file: `cat some-file.txt`
- go one folder up: `cd ..`

```
1 login as: frosch
2 frosch@analysis-01.compute.fhi.mpg.de's password:
3 Linux analysis-01 6.1.0-31-cloud-amd64 #1 SMP ...
4 Last login: Tue Feb 25 11:55:56 2025 from 141.14.136.106
5 (base) frosch@analysis-01:~$ ls
6 data      Documents  local      Pictures   Templates
7 Desktop   Downloads  Music      Public     Videos
8 (base) frosch@analysis-01:~$ cd Downloads/
9 (base) frosch@analysis-01:~/Downloads$ ls
10 some-file.txt
11 (base) frosch@analysis-01:~/Downloads$ cat some-file.txt
12 Some content
13 (base) frosch@analysis-01:~/Downloads$ cd ..
14 (base) frosch@analysis-01:~$
```




TERMINAL ACCESS VIA SSH

You have terminal / SSH access to all compute servers!

Be sure to connect to the machine you need (analysis-01, -02, -03, ...)!

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Open Putty

- Enter the address `analysis-01.compute.fhi.mpg.de`
- Click `Open`
(You can as well `Save` this session!)
- Enter your **username**, press `Enter`
- Enter your **password** (invisible), press `Enter`.

Enter any commands, e.g.:

- list the content of this folder: `ls`
- go into a folder: `cd Downloads`
- show the content of a file: `cat some-file.txt`
- go one folder up: `cd ..`

```
1 login as: frosch
2 frosch@analysis-01.compute.fhi.mpg.de's password:
3 Linux analysis-01 6.1.0-31-cloud-amd64 #1 SMP ...
4 Last login: Tue Feb 25 11:55:56 2025 from 141.14.136.106
5 (base) frosch@analysis-01:~$ ls
6 data      Documents  local      Pictures   Templates
7 Desktop   Downloads  Music      Public     Videos
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9 (base) frosch@analysis-01:~/Downloads$ ls
10 some-file.txt
11 (base) frosch@analysis-01:~/Downloads$ cat some-file.txt
12 Some content
13 (base) frosch@analysis-01:~/Downloads$ cd ..
14 (base) frosch@analysis-01:~$
```



TERMINAL ACCESS VIA SSH

You have terminal / SSH access to all compute servers!

Be sure to connect to the machine you need (analysis-01, -02, -03, ...)!

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Open Putty

- Enter the address `analysis-01.compute.fhi.mpg.de`
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Enter any commands, e.g.:

- list the content of this folder: `ls`
- go into a folder: `cd Downloads`
- show the content of a file: `cat some-file.txt`
- go one folder up: `cd ..`

```
1 login as: frosch
2 frosch@analysis-01.compute.fhi.mpg.de's password:
3 Linux analysis-01 6.1.0-31-cloud-amd64 #1 SMP ...
4 Last login: Tue Feb 25 11:55:56 2025 from 141.14.136.106
5 (base) frosch@analysis-01:~$ ls
6 data      Documents  local      Pictures   Templates
7 Desktop   Downloads  Music      Public     Videos
8 (base) frosch@analysis-01:~$ cd Downloads/
9 (base) frosch@analysis-01:~/Downloads$ ls
10 some-file.txt
11 (base) frosch@analysis-01:~/Downloads$ cat some-file.txt
12 Some content
13 (base) frosch@analysis-01:~/Downloads$ cd ..
14 (base) frosch@analysis-01:~$
```



TERMINAL ACCESS VIA SSH

You have terminal / SSH access to all compute servers!

Be sure to connect to the machine you need (analysis-01, -02, -03, ...)!

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Open Putty

- Enter the address `analysis-01.compute.fhi.mpg.de`
- Click `Open`
(You can as well `Save` this session!)
- Enter your **username**, press `Enter`
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Enter any commands, e.g.:

- list the content of this folder: `ls`
- go into a folder: `cd Downloads`
- show the content of a file: `cat some-file.txt`
- go one folder up: `cd ..`

```
1 login as: frosch
2 frosch@analysis-01.compute.fhi.mpg.de's password:
3 Linux analysis-01 6.1.0-31-cloud-amd64 #1 SMP ...
4 Last login: Tue Feb 25 11:55:56 2025 from 141.14.136.106
5 (base) frosch@analysis-01:~$ ls
6 data      Documents  local      Pictures   Templates
7 Desktop   Downloads  Music      Public     Videos
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9 (base) frosch@analysis-01:~/Downloads$ ls
10 some-file.txt
11 (base) frosch@analysis-01:~/Downloads$ cat some-file.txt
12 Some content
13 (base) frosch@analysis-01:~/Downloads$ cd ..
14 (base) frosch@analysis-01:~$
```



TERMINAL ACCESS VIA SSH

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Open Putty

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- Enter your **username**, press `Enter`
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Enter any commands, e.g.:

- list the content of this folder: `ls`
- go into a folder: `cd Downloads`
- show the content of a file: `cat some-file.txt`
- go one folder up: `cd ..`

```
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2 frosch@analysis-01.compute.fhi.mpg.de's password:
3 Linux analysis-01 6.1.0-31-cloud-amd64 #1 SMP ...
4 Last login: Tue Feb 25 11:55:56 2025 from 141.14.136.106
5 (base) frosch@analysis-01:~$ ls
6 data      Documents  local      Pictures   Templates
7 Desktop   Downloads  Music      Public     Videos
8 (base) frosch@analysis-01:~$ cd Downloads/
9 (base) frosch@analysis-01:~/Downloads$ ls
10 some-file.txt
11 (base) frosch@analysis-01:~/Downloads$ cat some-file.txt
12 Some content
13 (base) frosch@analysis-01:~/Downloads$ cd ..
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```



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Be sure to connect to the machine you need (analysis-01, -02, -03, ...)!

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Open Putty

- Enter the address `analysis-01.compute.fhi.mpg.de`
- Click `Open`
(You can as well `Save` this session!)
- Enter your *username*, press `Enter`
- Enter your *password* (invisible), press `Enter`.

Enter any commands, e.g.:

- list the content of this folder: `ls`
- go into a folder: `cd Downloads`
- show the content of a file: `cat some-file.txt`
- go one folder up: `cd ..`

```
1 login as: frosch
2 frosch@analysis-01.compute.fhi.mpg.de's password:
3 Linux analysis-01 6.1.0-31-cloud-amd64 #1 SMP ...
4 Last login: Tue Feb 25 11:55:56 2025 from 141.14.136.106
5 (base) frosch@analysis-01:~$ ls
6 data      Documents  local      Pictures   Templates
7 Desktop   Downloads  Music      Public     Videos
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10 some-file.txt
11 (base) frosch@analysis-01:~/Downloads$ cat some-file.txt
12 Some content
13 (base) frosch@analysis-01:~/Downloads$ cd ..
14 (base) frosch@analysis-01:~$
```



FURTHER TOPICS & LINKS

MORE TRAINING MATERIAL

Visit root.compute.fhi.mpg.de/training

PPB WIKI | HPC

General Information.

FHI GITLAB | HPC DOCUMENTATION

Jupyterhub Wiki | Virtual Desktop Wiki | Storage Wiki

Questions, issues, needing help?

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