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Fakultät für Geowissenschaften,  
Geographie und Astronomie

# Bare metal, shells and clouds

## IT2Research - UPDATES

18. März 2024

M. Blaschek

PhD Seminar @ IMG Vienna



imgw

# What you can expect from this presentation

Hardware

How to  
use  
servers?

Data &  
Storage

Services  
@ ZID

Services  
@ IMG

Updates

Questions?  
Ask anytime –  
interrupt me





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# Bare metal

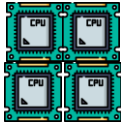
Hardware, VSC, ECMWF

# Bare metal @ Department – SRVX – JET – VSC Nodes

## SRVX1



- Arsenal
- 4x CPU
- Development Node
- **Teaching Node**
- Storage Node
  - 800 TB



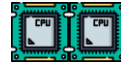
## SRVX8



## AURORA



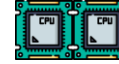
- Arsenal
- 2x CPU
- **Visual Node (VNC)**
- **Development Node**



## JET




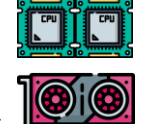
- Arsenal
- 2x Login (hub, vnc)
- 7x Compute CPU
- **Computing/Post Processing Cluster**
- Storage 3.5 PB Global Storage
- Scheduler (**slurm**)
- Planned: Extend num. Nodes + Storage



## VSC 4 / 5



- Arsenal
- **VSC4** - 5x Nodes
- **VSC5** – 11x Nodes
- VSC5 – 1x GPU
- **Computing Cluster**
- Shared HOME (200GB)
- Shared DATA (100TB)
- Scheduler (**slurm**)
- Projects can be requested (resources)
-  JETFS on VSC



# Other HPC that might be relevant for you



WEKEO

- Copernicus DIAS (Data & Info Access S.)
- Explore all Copernicus Data
- JupyterHub
- Limited Storage space
- Recipe: Explore what could be useful
- Sign up free.



ECMWF

- Bologna HPC
- Supervisor can get you access
- **MARS** Data archive



- Jupyter - [eodc.wolke.img.univie.ac.at](https://eodc.wolke.img.univie.ac.at)
- EODC – products (Sentinel, GPSRO, ERA5,...)



Leonardo

- April 2023
- Europe **2nd** HPC
- Proposals to VSC (Projects)





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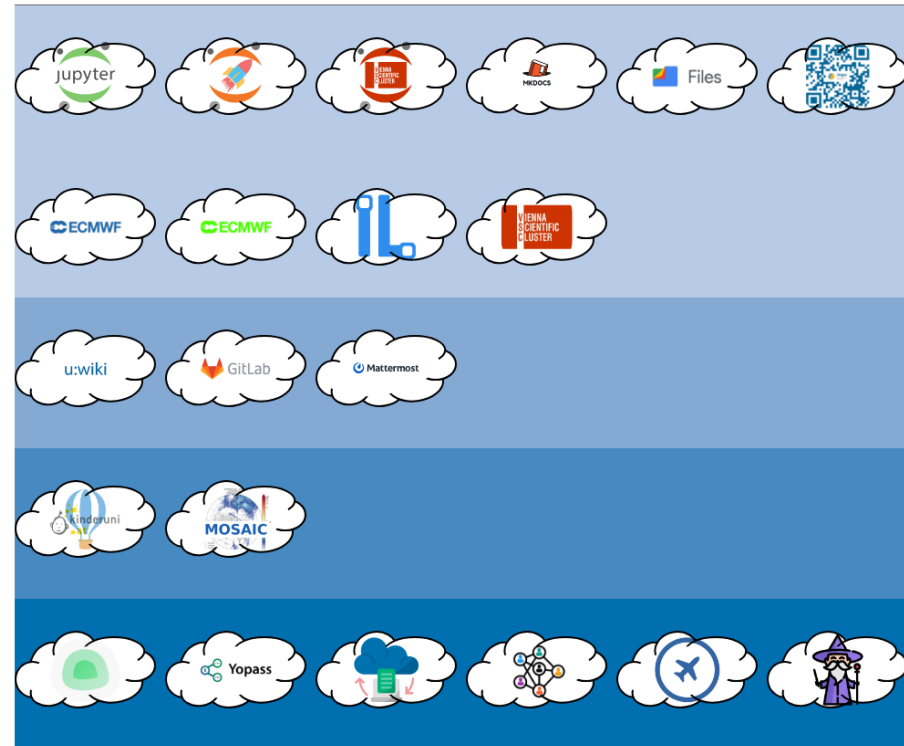
# Shells & tools

Starting point, Command line

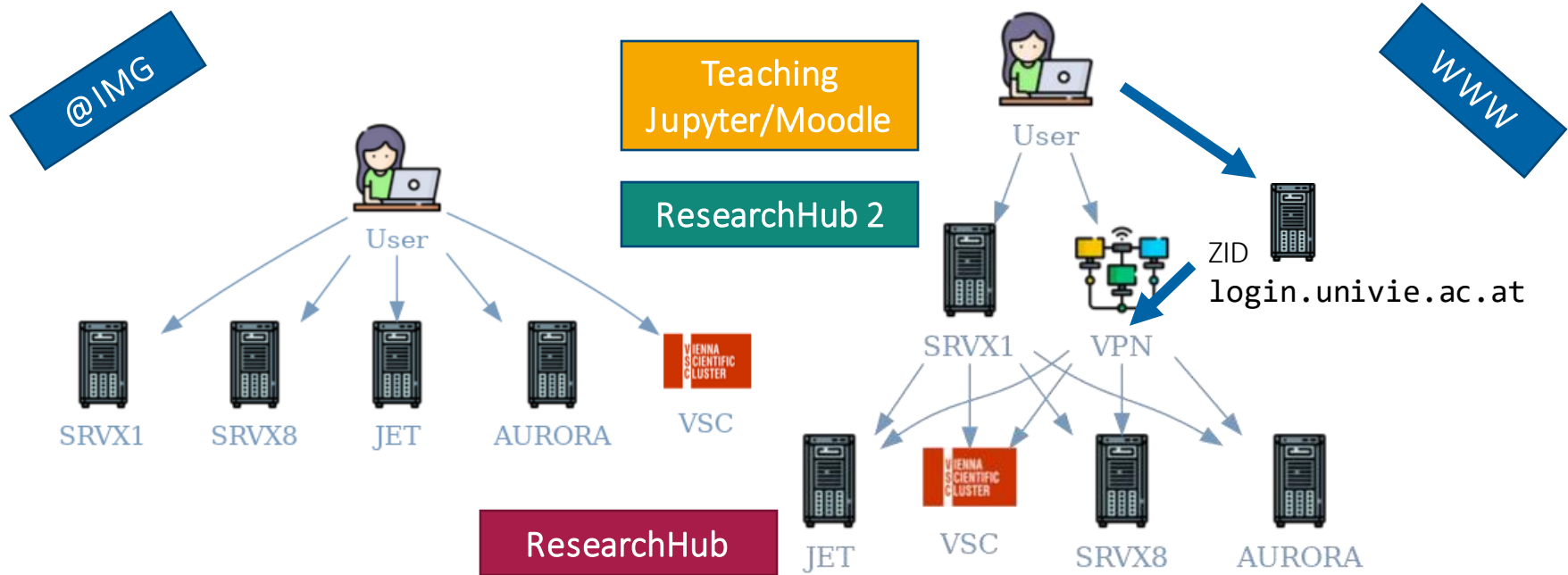


# Shells & tools – Wolke (cloud)

- Where to start? *Wolke*
- Where to go first? *Wolke*
- What can help you? *Wolke*
- <https://wolke.img.univie.ac.at>
- Server related issues?
  - Schedule
  - Status of Services



# Shells & tools – Access





# Shells & tools – Accounts

## 1. u:account

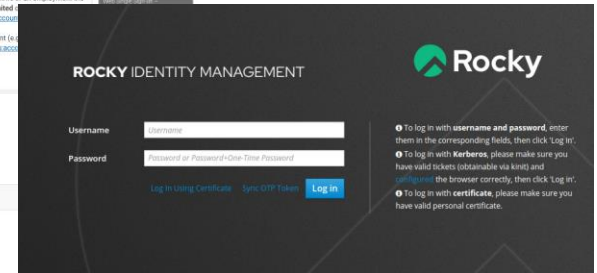
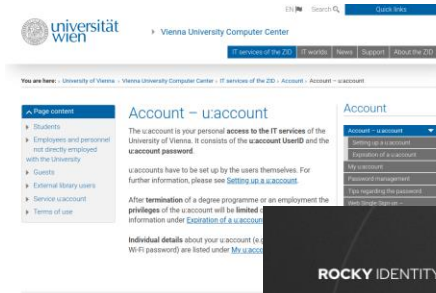
- All ZID services
- Jupyterhub @Moodle

## 2. w:account (Wolke IMG account)

- All servers
- Jupyterhub on JET

## ~~3. t:account TeachingHub~~

## 4. ECMWF account



Welcome to the High Performance Computer at the Institut of Meteorology and Geophysics.

Please login with your Jet credentials.

Sign in

Username:

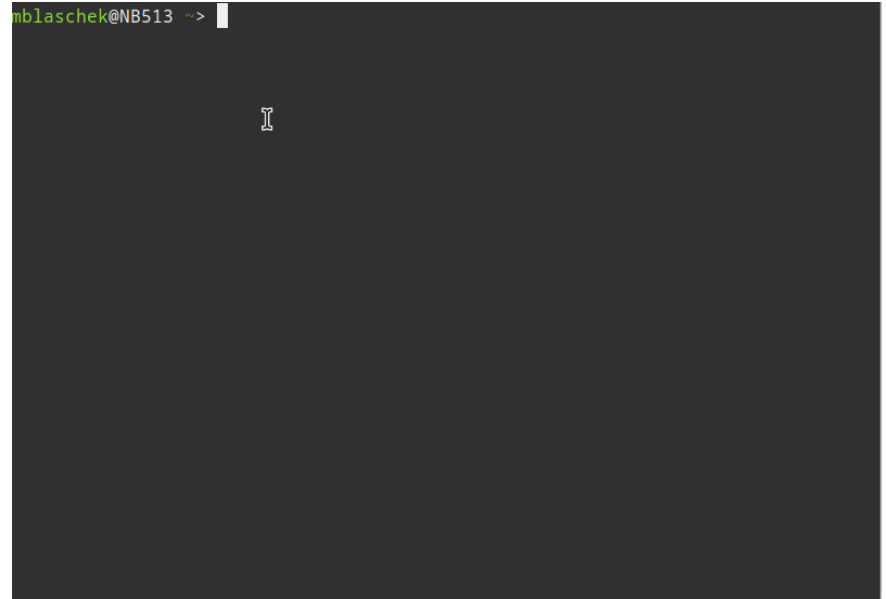
Password:

Sign in



# Shells & tools – userservices

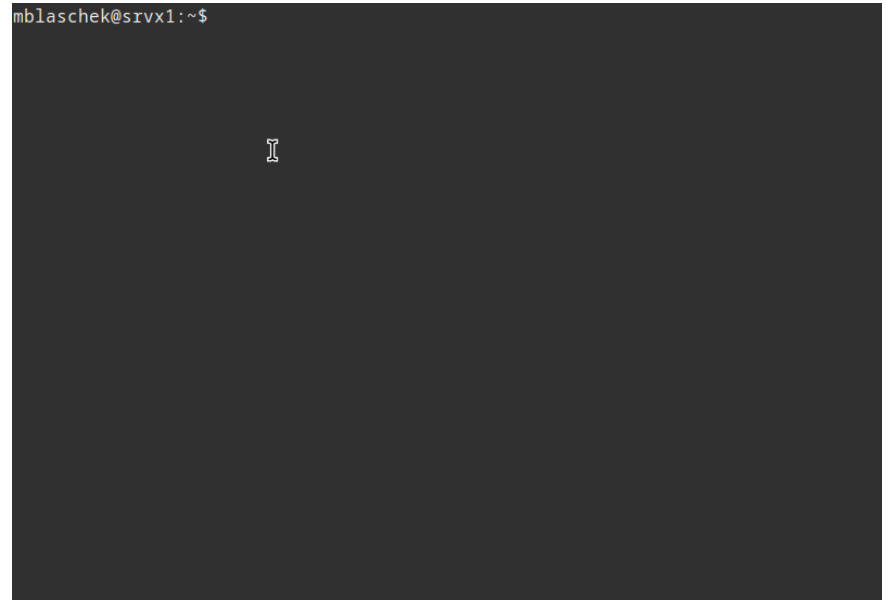
- **userservices** – collection of useful scripts
  - **filesender** – [ACOnet](#) 250 GB
  - **quota** – storage quota of user
  - ~~sshtools~~ – ssh agent manager
  - **transfersh** – send small files (<500 MB)
  - **ucloud** – upload to u:cloud
  - **yopass** – encrypt messages
  - **vnc** – Virtual desktop on SRVX8
  - **weather** – current weather info
  - **archive** – send off to ZID archive



# Shells & tools – userservices filesender

- **userservices** – collection of useful scripts
  - **filesender** – [ACOnet](#) 250 GB
  - **quota** – storage quota of user
  - **sshtools** – ssh agent manager
  - **transfersh** – send small files (<500 MB)
  - **ucloud** – upload to u:cloud
  - **yopass** – encrypt messages
  - **vnc** – Virtual desktop on SRVX8
  - **weather** – current weather info

```
mblaschek@srvx1:~$
```

A terminal window with a dark background. The prompt 'mblaschek@srvx1:~\$' is visible at the top left. A white cursor is positioned in the center of the screen.

# Shells & tools – userservices ~~sshtools~~

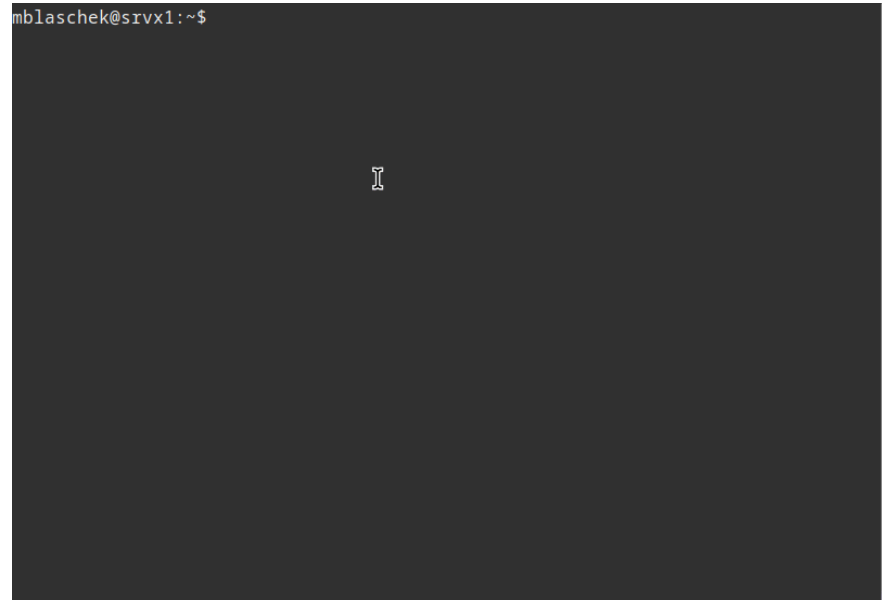
- **userservices** – collection of useful scripts
  - **filesender** – [ACOnet](#) 250 GB
  - **quota** – storage quota of user
  - ~~**sshtools**~~ – ssh agent manager
  - **transfersh** – send small files (<500 MB)
  - **ucloud** – upload to u:cloud
  - **yopass** – encrypt messages
  - **vnc** – Virtual desktop on SRVX8
  - **weather** – current weather info

```
mblaschek@srvx1:~$ exit
logout
Connection to srvx1.img.univie.ac.at closed.
mblaschek@NB513 ~>
```

# Shells & tools – userservices transfersh

- **userservices** – collection of useful scripts
  - **filesender** – [ACOnet](#) 250 GB
  - **quota** – storage quota of user
  - **sshtools** – ssh agent manager
  - **transfersh** – send small files (<500 MB)
  - **ucloud** – upload to u:cloud
  - **yopass** – encrypt messages
  - **vnc** – Virtual desktop on SRVX8
  - **weather** – current weather info

```
mblaschek@srvx1:~$
```

A terminal window with a dark background. The prompt 'mblaschek@srvx1:~\$' is visible at the top left. A white cursor is positioned in the center of the terminal area.

# Shells & tools – userservices vnc

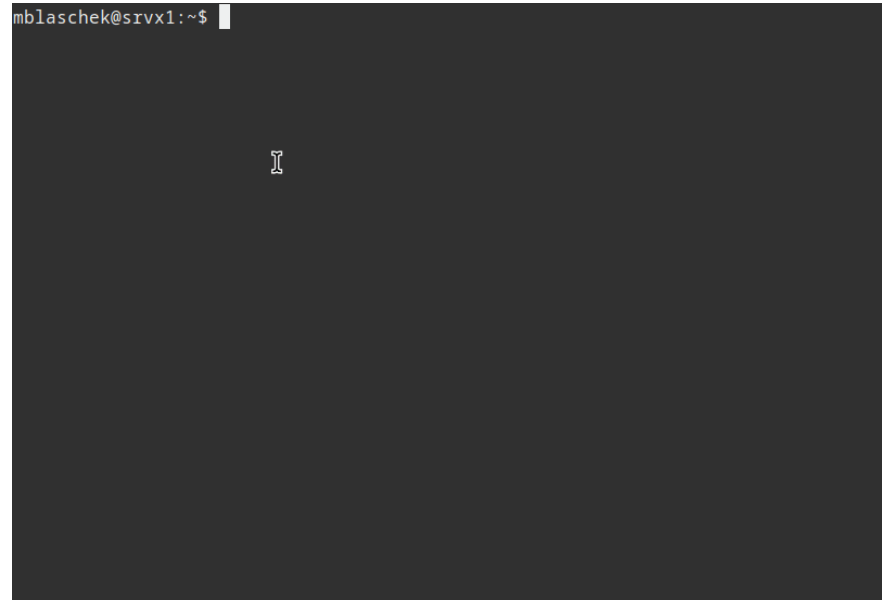
- **userservices** – collection of useful scripts
  - **filesender** – [ACOnet](#) 250 GB
  - **quota** – storage quota of user
  - **sshtools** – ssh agent manager
  - **transfersh** – send small files (<500 MB)
  - **ucloud** – upload to u:cloud
  - **yopass** – encrypt messages
  - **vnc** – Virtual desktop on SRVX8
  - **weather** – current weather info

```
mblaschek@srvx1:~$  
  
I
```

# Shells & tools – user support

- Environment modules on all servers + HPCs
  - Dynamic loading of different versions of the same library/software
- `module av`
- `module list`
- `module load <mod name>`
- `module purge`

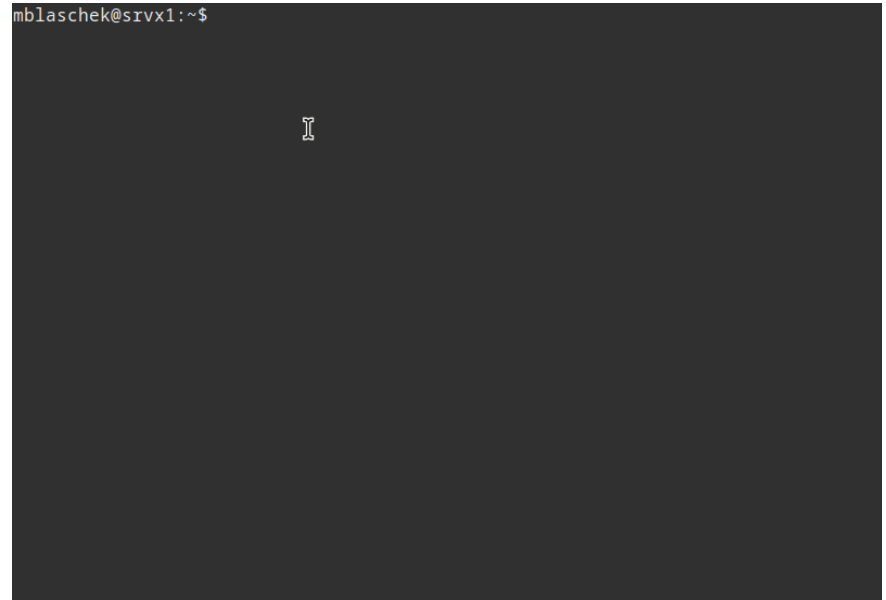
```
mblaschek@srvx1:~$
```

A terminal window with a dark background. The prompt 'mblaschek@srvx1:~\$' is visible at the top left. A white cursor is positioned in the center of the terminal area.



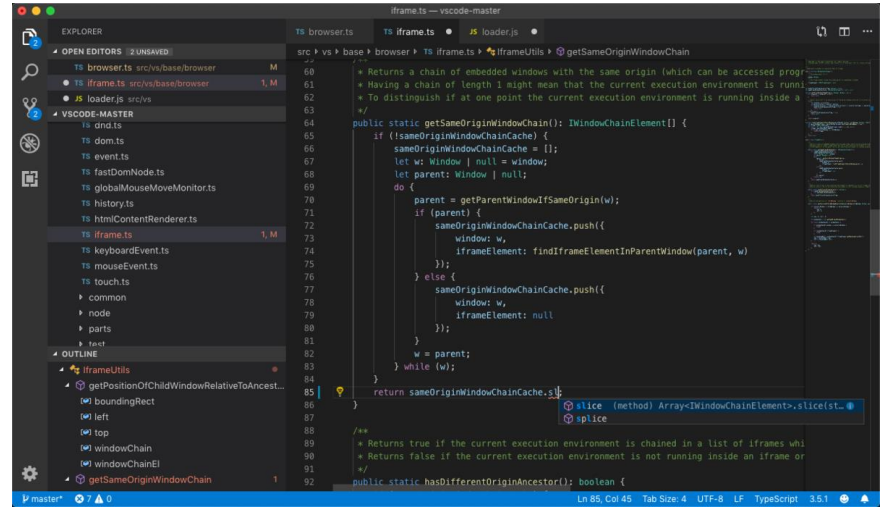
# Shells & tools – user support

- Most users have bash (`chsh -l`)
- Easy for beginners: `fish`
- Shells use configuration files, e.g. `.bashrc`, `.cshrc`, ...
- Scripts can use all kind of shells
  - `#!/bin/bash`
- Cause of trouble
  - Module load in `.bashrc`, create `alias`  
`mymod="module load <modules>"`

A terminal window with a dark background. The prompt is `mblaschek@srvx1:~$`. A white cursor is positioned in the center of the terminal.

# Shells & tools – user support - recommendations

- Editors: **vim**, nano
- Dev Environment: **VSCode**, Code OSS
  - Extensions: Remote SSH, Dev Containers, Python, Notebooks, Modern Fortran, ...
  - Git fully integrated
- Python: build your own environment
  - Use conda or **micromamba**
  - Install packages, create environment file for a working environment (backup)
  - Add as a kernel to TeachingHub/ResearchHub

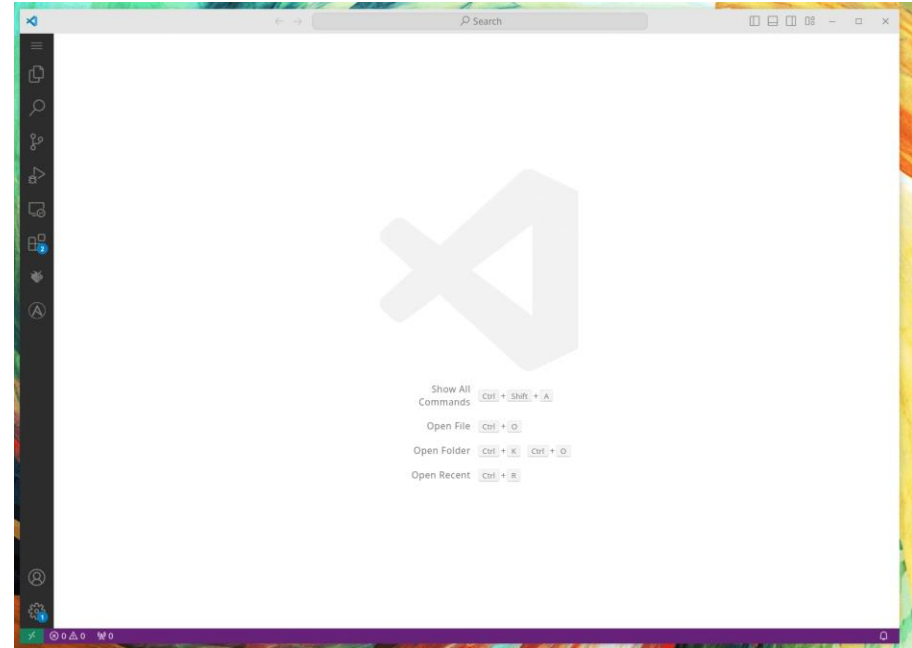


```
ifframe.ts — vscode-master
EXPLORER
OPEN EDITORS (UNSAVED)
  browser.ts src/vs/base/browser M
  iframe.ts src/vs/base/browser 1, M
  loader.ts src/vs 62
VSCODE-MASTER
  dnd.ts 64
  dom.ts 65
  event.ts 66
  fastDomNode.ts 67
  globalMouseMoveMonitor.ts 68
  history.ts 69
  htmlContentRenderer.ts 70
  iframe.ts 71, M
  keyboardEvent.ts 72
  mouseEvent.ts 73
  touch.ts 74
  common 75
  parts 76
  test 77
  OUTLINE 78
    iframeUtils 79
    getPositionOfChildWindowRelativeToAncestor... 80
    boundingRect 81
    left 82
    top 83
    windowChain 84
    windowChainEl 85
    getSameOriginWindowChain 86
    hasDifferentOriginAncestor 87
    88
    89
    90
    91
    92
  1

src > vs > base > browser > iframe.ts > iframeUtils > getSameOriginWindowChain
71
72
73
74
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89
90
91
92
* Returns a chain of embedded windows with the same origin (which can be accessed prog
* Having a chain of length 1 might mean that the current execution environment is runni
* To distinguish if at one point the current execution environment is running inside a
*/
public static getSameOriginWindowChain(): IWindowChainElement[] {
  if (!sameOriginWindowChainCache) {
    sameOriginWindowChainCache = [];
    let w: Window | null = window;
    let parent: Window | null;
    do {
      parent = getParentWindowIfSameOrigin(w);
      if (parent) {
        sameOriginWindowChainCache.push({
          window: w,
          iframeElement: findIframeElementInParentWindow(parent, w)
        });
      } else {
        sameOriginWindowChainCache.push({
          window: w,
          iframeElement: null
        });
      }
      w = parent;
    } while (w);
  }
  return sameOriginWindowChainCache.slice(
    // slice (method) Array<IWindowChainElement>.slice(st...
    // splice
  );
}
* Returns true if the current execution environment is chained in a list of iframes whi
* Returns false if the current execution environment is not running inside an iframe or
*/
public static hasDifferentOriginAncestor(): boolean {
  ln 85, Col 45 Tab Size: 4 UTF-8 LF TypeScript 3.5.1
```

# Shells & tools – VSCode

- VSCode (**Microsoft**, Open source)
- Extensions:
  - Remote Development (WSL, DevC, **SSH**, **Tunnels**)
  - Remote Explorer (**.ssh/config**)
  - Python/Jupyter
  - Fortran
  - Prettier - Code Formatter
  - Shell Syntax
  - Git graph (git branches/ merges,...)
  - Jupyterhub (remote kernel execution)



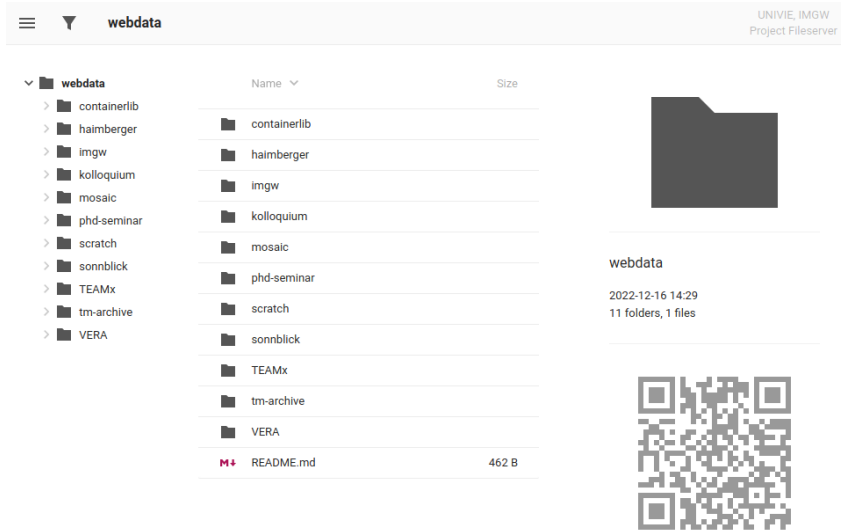


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# clouds and services

@IMG, @ZID, ...

# Clouds and services – webdata



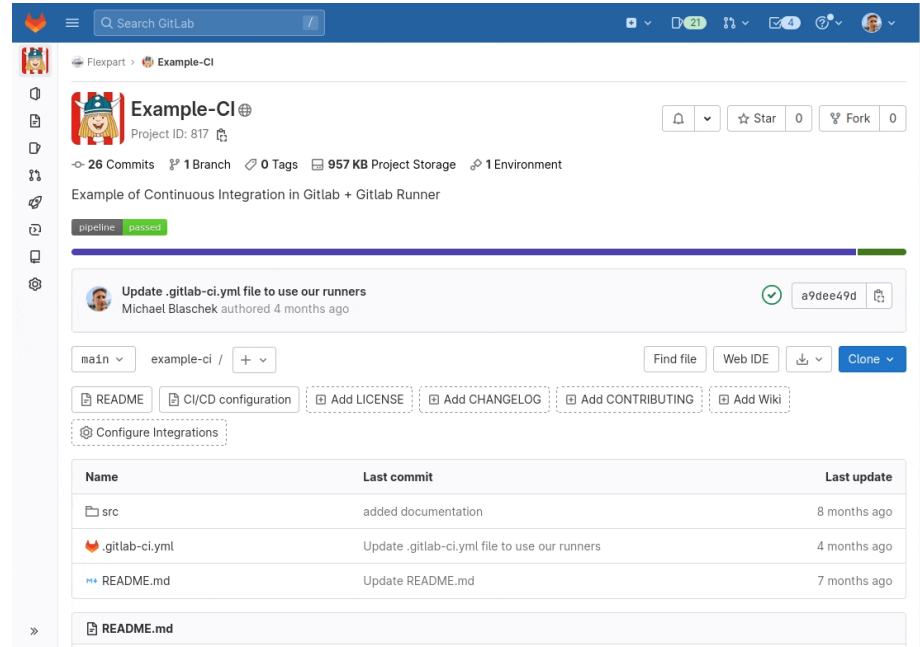
The screenshot shows a file manager interface for a 'Project Fileserver' (UNIVIE, IMGW). The main view displays a directory tree on the left and a list of files and folders in the center. The 'webdata' directory is expanded, showing sub-directories like 'containerlib', 'haimberger', 'imgw', 'kolloquium', 'mosaic', 'phd-seminar', 'scratch', 'sonnblick', 'TEAMx', 'tm-archive', and 'VERA'. A 'README.md' file is also listed with a size of 462 B. On the right, a preview of the 'webdata' folder is shown, including its creation date (2022-12-16 14:29) and contents (11 folders, 1 file). A QR code is displayed below the preview.

Name	Size
containerlib	
haimberger	
imgw	
kolloquium	
mosaic	
phd-seminar	
scratch	
sonnblick	
TEAMx	
tm-archive	
VERA	
README.md	462 B

- Wolke > files
- `/mnt/scratch/webdata`
- Request a directory or create one in scratch
- Authentication can be requested too  
user:pwd
- Accessible to everybody
- **Please Clean up!!!**

# Clouds and services – gitlab

- Continuous integration (CI) and development
  - Code testing
  - Deployment
  - Development in groups
- 2 Runners (IMGW, Flexpart, ... Groups)
- Example: <https://gitlab.phaidra.org/imgw/example-ci>
- Is not free
- Optional: prebuild images

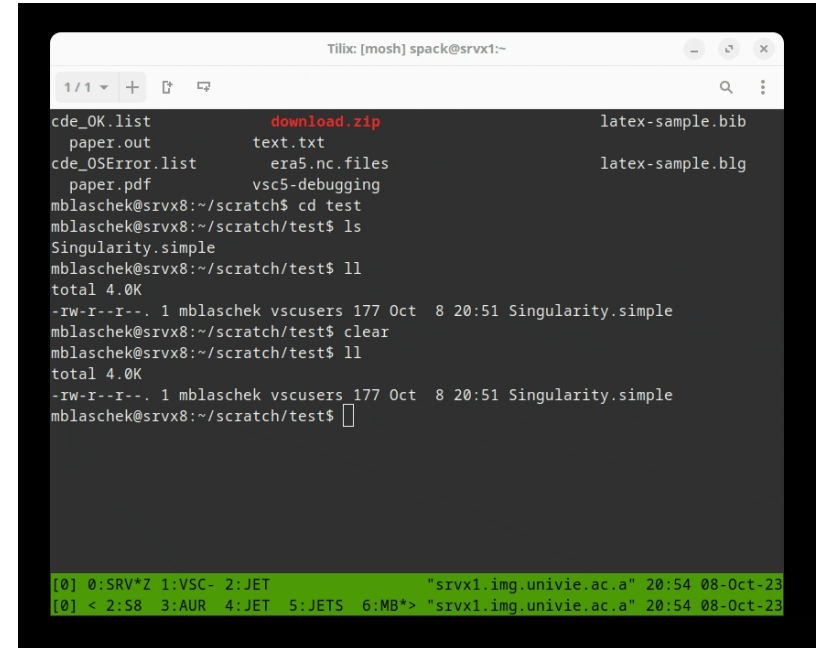


The screenshot shows the GitLab web interface for a project named "Example-CI". The interface includes a search bar at the top, a navigation menu on the left, and a main content area. The main content area displays the project name "Example-CI" with a Project ID of 817. Below this, there are statistics for 26 Commits, 1 Branch, 0 Tags, 957 KB Project Storage, and 1 Environment. A pipeline status bar shows "pipeline: passed". A commit message "Update .gitlab-ci.yml file to use our runners" by Michael Blaschek is displayed, along with a commit hash "a9dee49d". Below the commit, there are buttons for "Find file", "Web IDE", "Download", and "Clone". A table of files is shown, including "src", ".gitlab-ci.yml", and "README.md".

Name	Last commit	Last update
src	added documentation	8 months ago
.gitlab-ci.yml	Update .gitlab-ci.yml file to use our runners	4 months ago
README.md	Update README.md	7 months ago

# Cloud and services – apptainer / singularity

- Deploy your work in a container
- Build once & run everywhere
- **Every user** can now use **fakeroot** to build containers on our servers
- Integrate with gitlab-ci
- Publish on IMGW  
registry: [harbor.wolke.img.univie.ac.at](https://harbor.wolke.img.univie.ac.at)
- experimental



The image shows a terminal window titled 'Tilix: [mosh] spack@srvx1:~'. The terminal output shows the following sequence of commands and results:

```
cde_OK.list          download.zip          latex-sample.bib
  paper.out          text.txt
cde_OSError.list    era5.nc.files        latex-sample.blg
  paper.pdf          vsc5-debugging
mblaschek@srvx8:~/scratch$ cd test
mblaschek@srvx8:~/scratch/test$ ls
Singularity.simple
mblaschek@srvx8:~/scratch/test$ ll
total 4.0K
-rw-r--r--. 1 mblaschek vscusers 177 Oct  8 20:51 Singularity.simple
mblaschek@srvx8:~/scratch/test$ clear
mblaschek@srvx8:~/scratch/test$ ll
total 4.0K
-rw-r--r--. 1 mblaschek vscusers 177 Oct  8 20:51 Singularity.simple
mblaschek@srvx8:~/scratch/test$
```

At the bottom of the terminal, there are two green status lines:

```
[0] 0:SRV*Z 1:VSC- 2:JET          "srvx1.img.univie.ac.a" 20:54 08-Oct-23
[0] < 2:S8  3:AUR  4:JET  5:JETS  6:MB*> "srvx1.img.univie.ac.a" 20:54 08-Oct-23
```

# Clouds and services – ZID

- **u:cloud** for your files (50 Gb, backup)
- **MS365** office (**web** or windows)
- **Overleaf** – Online Latex
- **Gitlab** on Phaidra + **Mattermost**
- **VPN** or login or srvx1
- **u:wiki** - Tutorials, Teaching, Groups, Templates, ...






# Resources @IMG


# Resources – Teaching

- Lots of information in [u:wiki – Tutorials – Teaching](#)
- Moodle (u:account)
- **TeachingHubv2** for your course
- Student Response System (SRS)
  - [srs.univie.ac.at](https://srs.univie.ac.at) (feedback, questions, live)


WS2023-280320-1 / Übungen / JupyterHub / Einstellungen

 EXTERNES TOOL  
**JupyterHub**





Externes Tool   Einstellungen   Mehr ▾


 **Externes Tool in Übungen bearbeiten** Alles aufklappen


▾ **Allgemeines**

Name der Aktivität 

Mehr anzeigen ...

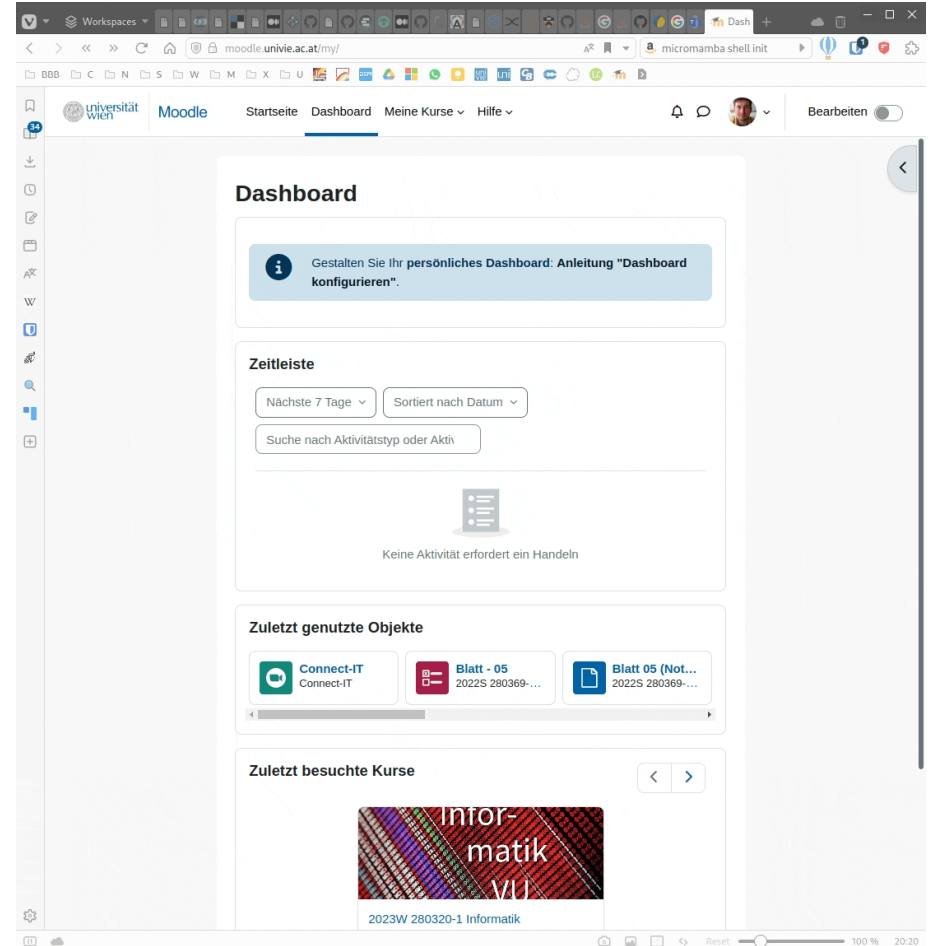
Vorkonfiguriertes Tool     

Tool-URL 

 Tool-Konfiguration verwenden: Jupyterhub (Meteorologie)

# Resources – Jupyter

- Jupyter Notebook Server (Hub):
  - ~~SRVX1~~ [teachinghub.wolke.img.univie.ac.at](https://teachinghub.wolke.img.univie.ac.at)
    - ResearchHub like on SRVX1
  - Teaching + Moodle (login)
    - SPL28
  - JET [jupyter.wolke.img.univie.ac.at](https://jupyter.wolke.img.univie.ac.at)
  - VSC Hub [jupyterhub.vsc.ac.at](https://jupyterhub.vsc.ac.at)
  - WEkEO [wekeo.eu](https://wekeo.eu)
  - EODC [eodc.wolke.img.univie.ac.at](https://eodc.wolke.img.univie.ac.at)
- Kernels with different python versions, packages
- Notebooks - Documentation + Code



Workspaces | moodle.univie.ac.at/my/ | micromamba shell init

universität wien Moodle Startseite Dashboard Meine Kurse Hilfe

### Dashboard

Gestalten Sie Ihr **persönliches Dashboard**. Anleitung "Dashboard konfigurieren".

#### Zeitleiste

Nächste 7 Tage | Sortiert nach Datum

Suche nach Aktivitätstyp oder Akti

Keine Aktivität erfordert ein Handeln

#### Zuletzt genutzte Objekte

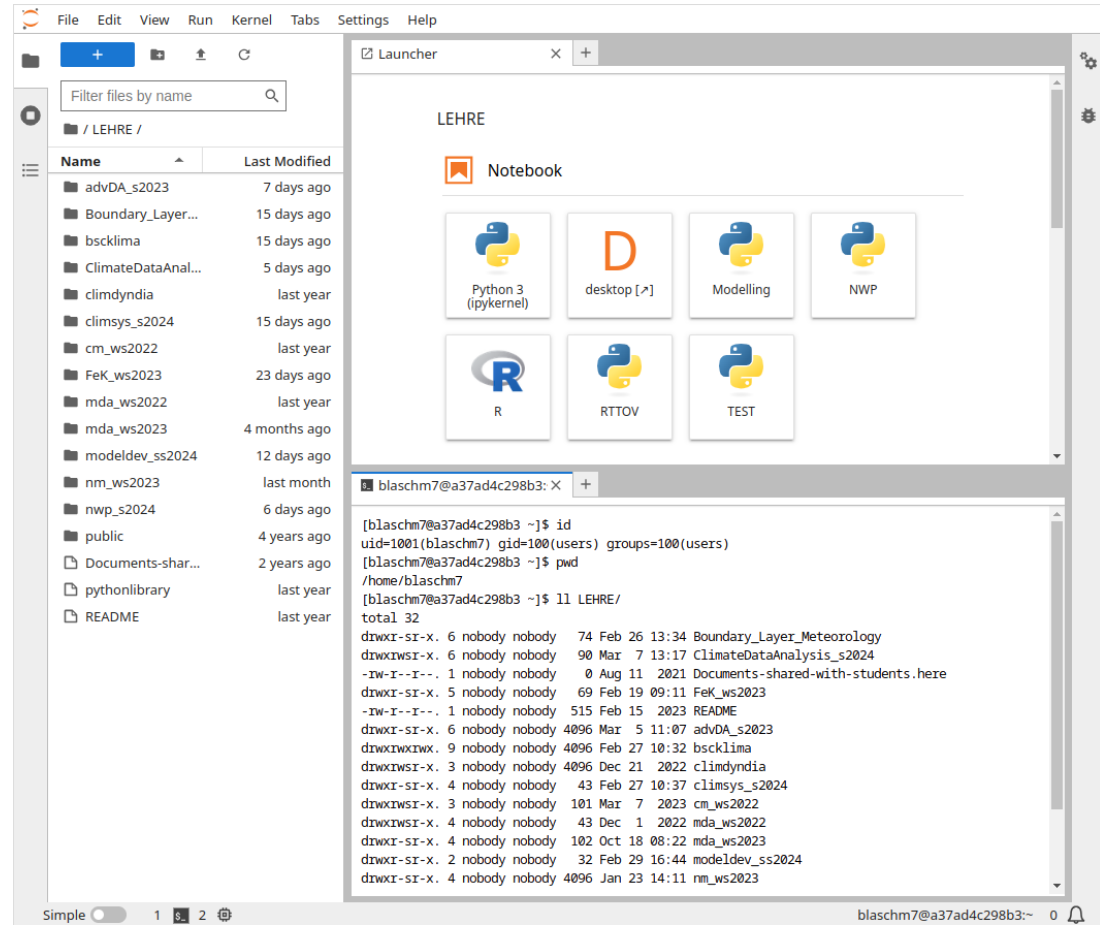
Connect-IT | Blatt - 05 | Blatt 05 (Not...

#### Zuletzt besuchte Kurse

Informatik | 2023W 280320-1 Informatik

# Working with the Moodle Jupyter Hub (TEACHING )

- All SPL28 students/lecturers have access
- $\$HOME/LEHRE$  maps to `/mnt/students/lehre` on SRVX1 (read only)
- SRVX1 user != teaching hub user
- Transfer files (`scp`, download) or userservices transfersh [file] + `wget`
- Purge in September (how to communicate to users?)



File Edit View Run Kernel Tabs Settings Help

Filter files by name

/ LEHRE /

Name	Last Modified
advDA_s2023	7 days ago
Boundary_Layer...	15 days ago
bscklima	15 days ago
ClimateDataAnal...	5 days ago
climdyndia	last year
climsys_s2024	15 days ago
cm_ws2022	last year
FeK_ws2023	23 days ago
mda_ws2022	last year
mda_ws2023	4 months ago
modeldev_ss2024	12 days ago
nm_ws2023	last month
nwp_s2024	6 days ago
public	4 years ago
Documents-shar...	2 years ago
pythonlibrary	last year
README	last year

Launcher

LEHRE

Notebook

Python 3 (ipykernel) desktop [^] Modelling NWP

R RTTOV TEST

```
[blaschm7@a37ad4c298b3 ~]$ id
uid=1001(blaschm7) gid=100(users) groups=100(users)
[blaschm7@a37ad4c298b3 ~]$ pwd
/home/blaschm7
[blaschm7@a37ad4c298b3 ~]$ ll LEHRE/
total 32
drwxr-xr-x. 6 nobody nobody 74 Feb 26 13:34 Boundary_Layer_Meteorology
drwxrwsr-x. 6 nobody nobody 90 Mar  7 13:17 ClimateDataAnalysis_s2024
-rw-r--r--. 1 nobody nobody  0 Aug 11 2021 Documents-shared-with-students_here
drwxr-xr-x. 5 nobody nobody 69 Feb 19 09:11 FeK_ws2023
-rw-r--r--. 1 nobody nobody 515 Feb 15 2023 README
drwxr-xr-x. 6 nobody nobody 4096 Mar  5 11:07 advDA_s2023
drwxrwxrwx. 9 nobody nobody 4096 Feb 27 10:32 bscklima
drwxrwsr-x. 3 nobody nobody 4096 Dec 21 2022 climdyndia
drwxr-xr-x. 4 nobody nobody  43 Feb 27 10:37 climsys_s2024
drwxrwsr-x. 3 nobody nobody 101 Mar  7 2023 cm_ws2022
drwxrwsr-x. 4 nobody nobody  43 Dec  1 2022 mda_ws2022
drwxr-xr-x. 4 nobody nobody 102 Oct 18 08:22 mda_ws2023
drwxr-xr-x. 2 nobody nobody  32 Feb 29 16:44 modeldev_ss2024
drwxr-xr-x. 4 nobody nobody 4096 Jan 23 14:11 nm_ws2023
```

Simple 1 2

blaschm7@a37ad4c298b3:~ 0



# Resources – Documentation

- Wolke – [documentation](#)
- Gitlab – IMGW Group
  - Computer Resources
    - Create an issue if you have something that is not working
  - Slurm
  - Singularity
- Wiki – Tutorials / HPC Resources information



# Resources – People

- **You can ask people to help you (no shame)**
- e.g.
  - ~~IT – Maximilian Meindl (ICON on JET/VSC)~~
  - IT – Michael Blaschek (HPC, Python, CI, Fortran, ...)
- Experts
  - Leopold Haimberger (Python, Fortran, ...)
  - Stefano Serafin (WRF, Python, Post processing, ...)
  - Marina Dütsch (Fortran, Python, Post processing, ...)
  - Lukas Brunner (Climate models, Post processing, ...)
- Many more experts here at the department
- Training courses @ VSC, PRACE training, Copernicus Training
- Could ask for a training course on a specific topic and organize that @IMG or a Hackaton



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# rules

Really ???





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# rules

YES

# Multi user systems need rules.

## Servers

---

- Storage **Quotas**
- JET job queuing (**fairshare** 🐿)
- VSC4 (5 Nodes) **HOME**
- VSC5 (11 Nodes) **file limits**
- Huge development work on
  - SRVX1, AURORA, JET01, JET02
- Long lasting jobs? > queue

## Interaction

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- Keep your credentials **private**
- **Change** your passwords (90d)
- Use **ssh-keys** in IPA
- *Your HOME shall be yours alone!*
- `drwx----- mblaschek users mblaschek`
- **Clean up your temp files**
- **Scratch is not going to be there forever!**
- **HOME is limited**







## Shared data

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- **/data**
- **/scratch/shared**
- **/jetfs/shared-data**
- **Respect other users**
- **Write a documentation**
- Give access to groups (met-..., geo-...)
- JET is shared on VSC
  - **/gpfs/jetfs**



# Communication is keen

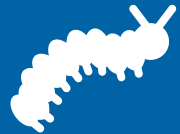
1. Check documentation (*talk to yourself*)  
2. Ask a colleague (*talk to another person*)  
3. Ask IT (*talk to a group*)  

# Contact IT

VSC related? >> Me

Server related? >> Me

Everything else/safe option >> [it.img-wien@univie.ac.at](mailto:it.img-wien@univie.ac.at) or mattermost – bugs





universität  
wien

# Questions?

PhD seminar

Bare metal, shells and clouds – MB

18.3.2024

On the wiki:  
tutorials – Computing

