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Fakultät für Geowissenschaften,  
Geographie und Astronomie

# Bare metal, shells and clouds

## IT2Research

9. Oktober 2023

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

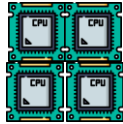
Hardware, VSC, ECMWF

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

## SRVX1



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



- 400 TB (users)
- 400 TB (scratch)

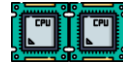
## SRVX8



## AURORA



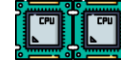
- Arsenal
- 2x CPU
- **Visual Node (VNC)**
- Development Node



## JET



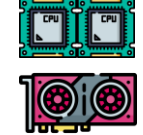
- Arsenal
- 2x Login
- 7x Compute CPU
- **Computing/Post Processing Cluster**
- Storage 3.5 PB Global Storage
- Scheduler (**slurm**)
- Planned: Extend num. Nodes + Storage



## VSC 4 / 5



- Arsenal
- **VSC4** - 5x CPU
- **VSC5** – 11x CPU
- 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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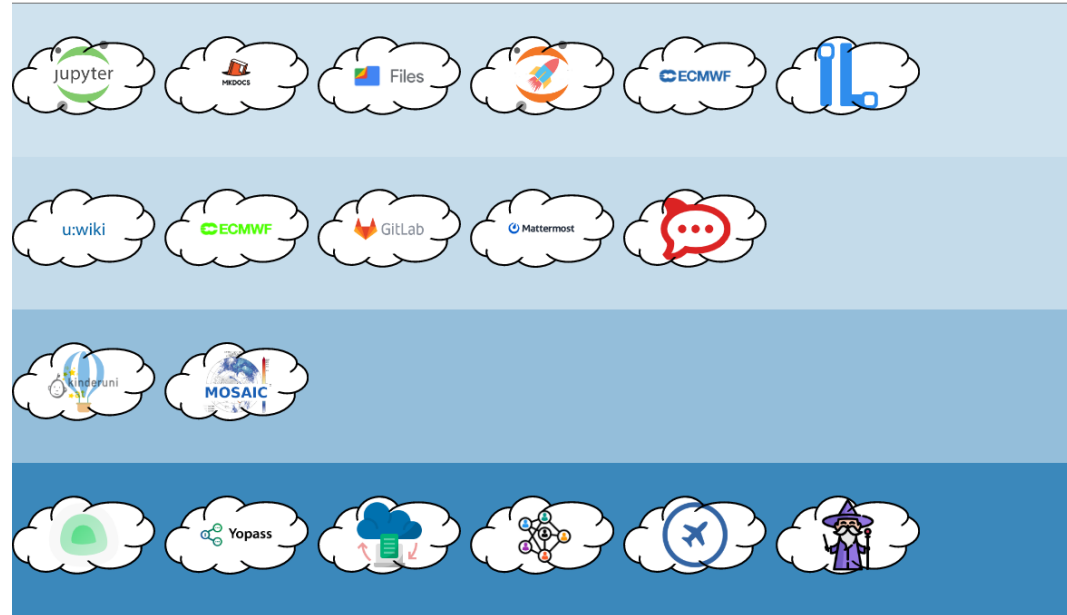
# Shells & tools

Starting point, Command line

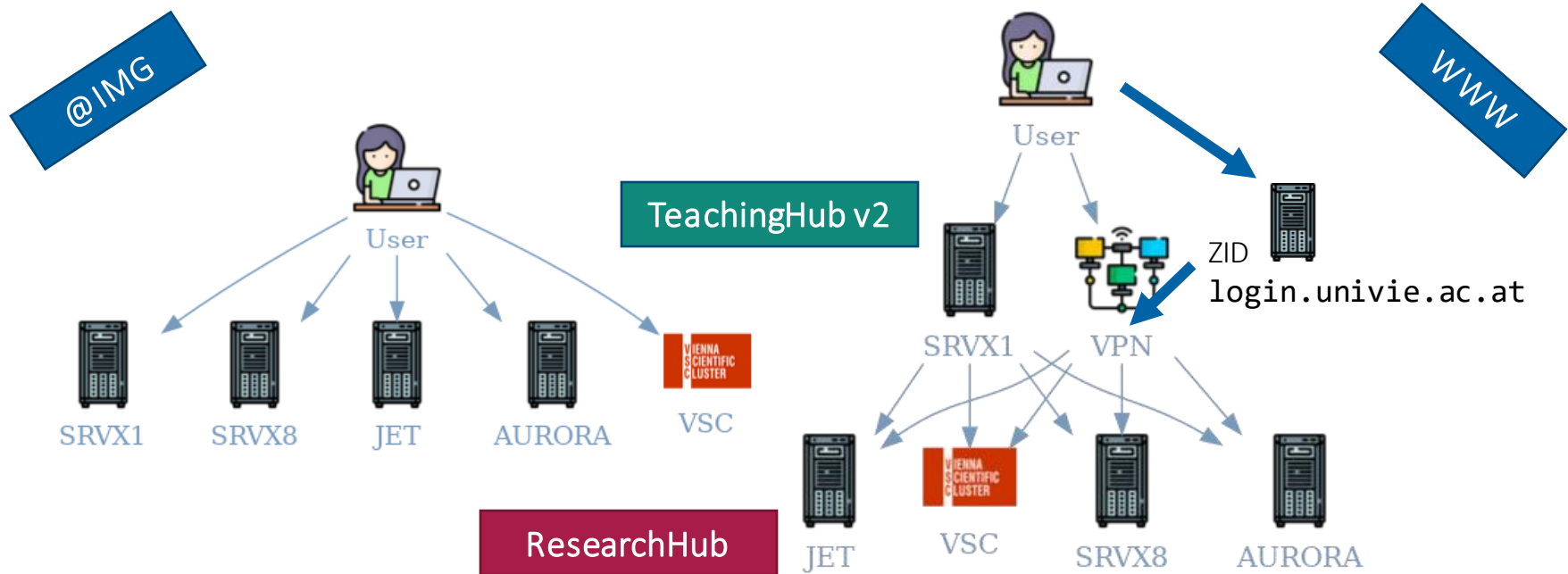


# Shells & tools – Wolke (cloud)

- 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

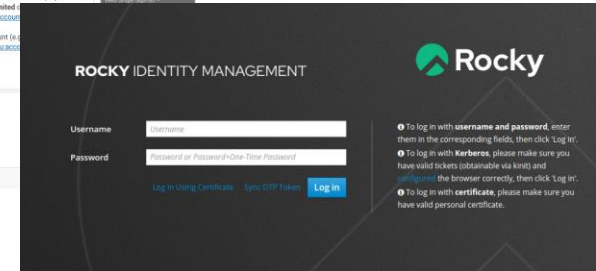
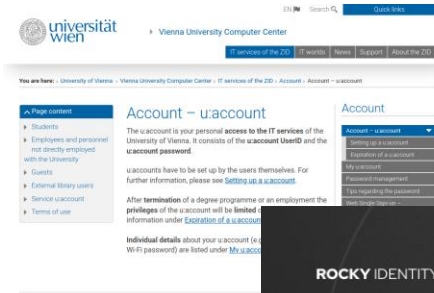
- All ZID services
- Jupyterhub @Moodle

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

- All servers
- Jupyterhub on JET

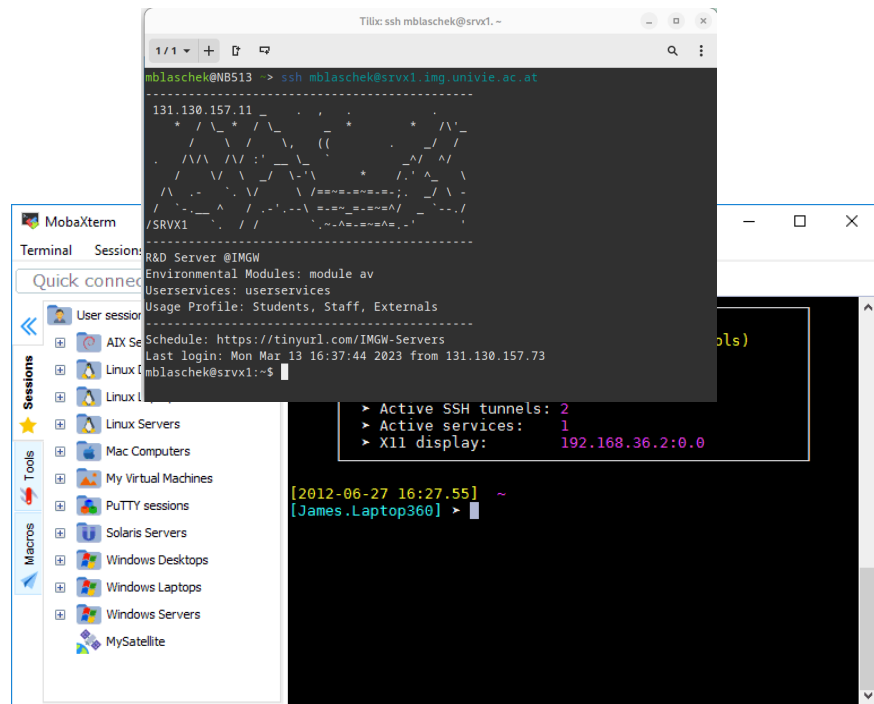
## 3. ~~t:account TeachingHub~~

## 4. ECMWF account



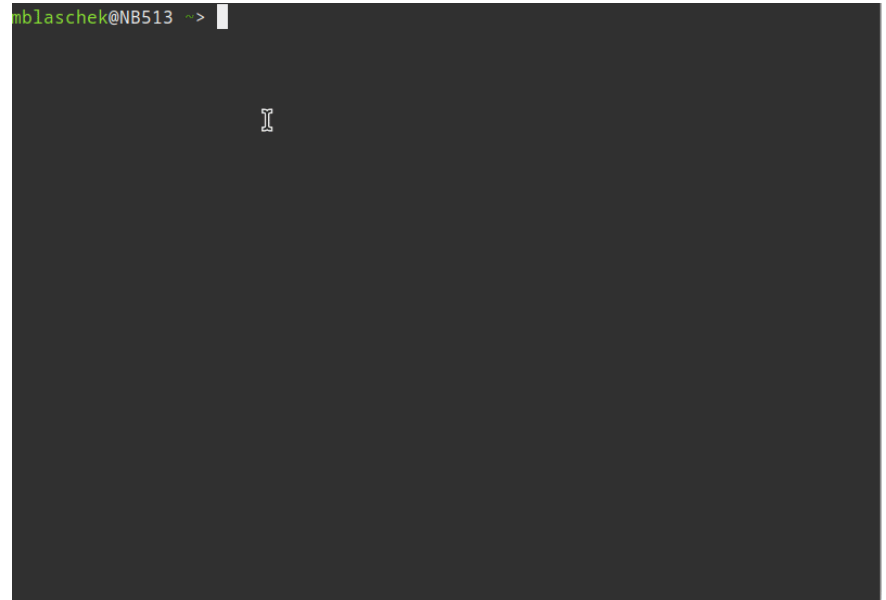
# Shells & tools – Connection 101

- Command line way:
  - Linux (**ssh**, **sftp**, ...)
  - Windows (MobaXterm (**ssh**, **sftp**, **vnc**), **ssh** client)
- Visual ways:
  - **Browser**, JupyterHub (srvx1, jet02, VSC, WEKEO, ECMWF, EODC)
  - **VNC**, Graphical Linux Server (srvx8, aurora, jet01)



# Shells & tools – userservices

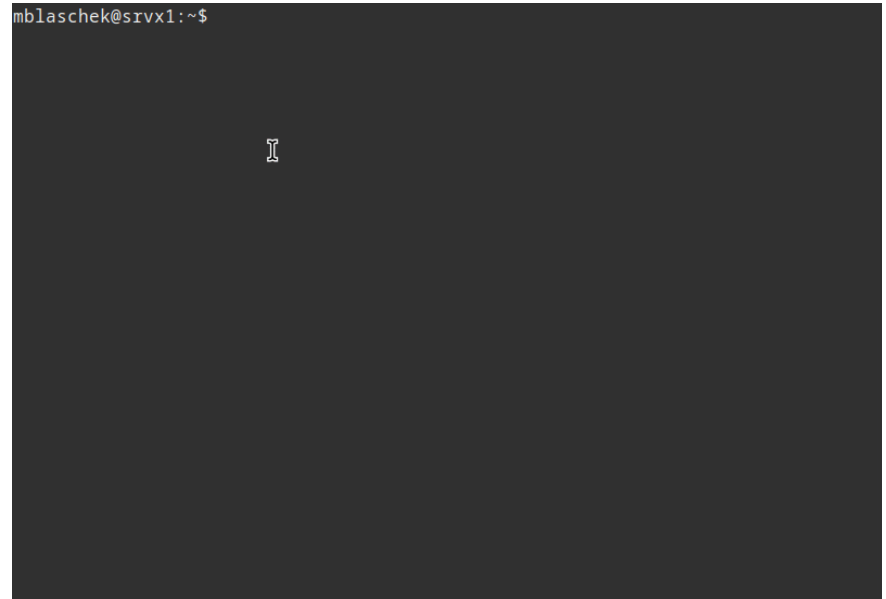
- **userservices** – collection of useful scripts
  - **filesender** – [ACOnet](#) 250 GB
  - **quota** – storage quota of user
  - **sshtools** – ssh agent manager
  - **transfersh** – send small files (<500 MB)
  - **ucloud** – upload to u:cloud
  - **yopass** – encrypt messages
  - **vnc** – Virtual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



# Shells & tools – userservices filesender

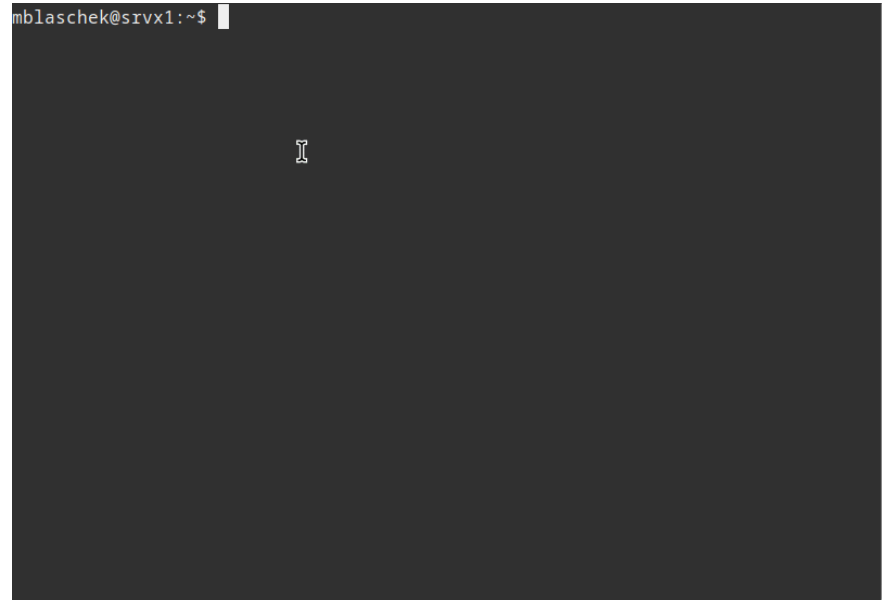
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```
mblaschek@srvx1:~$
```

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 sstools

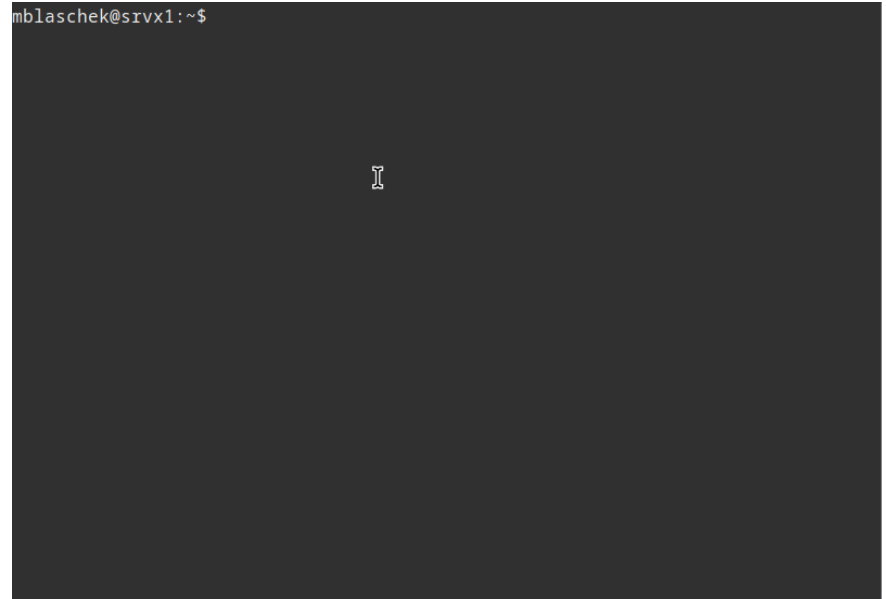
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# Shells & tools – userservices transfersh

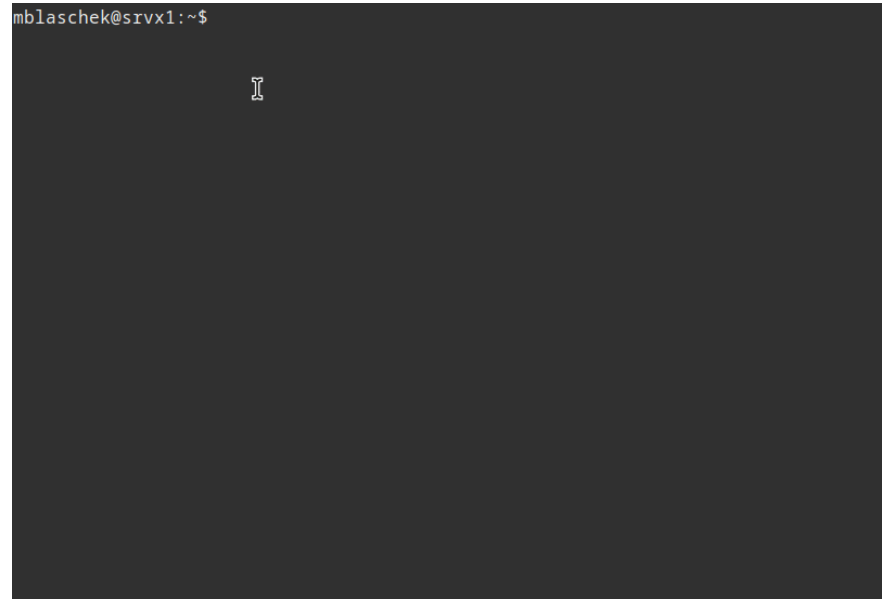
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  - **yopass** – encrypt messages
  - **vnc** – Virtual desktop on SRVX8
  - **weather** – current weather info

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

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

# Shells & tools – userservices vnc

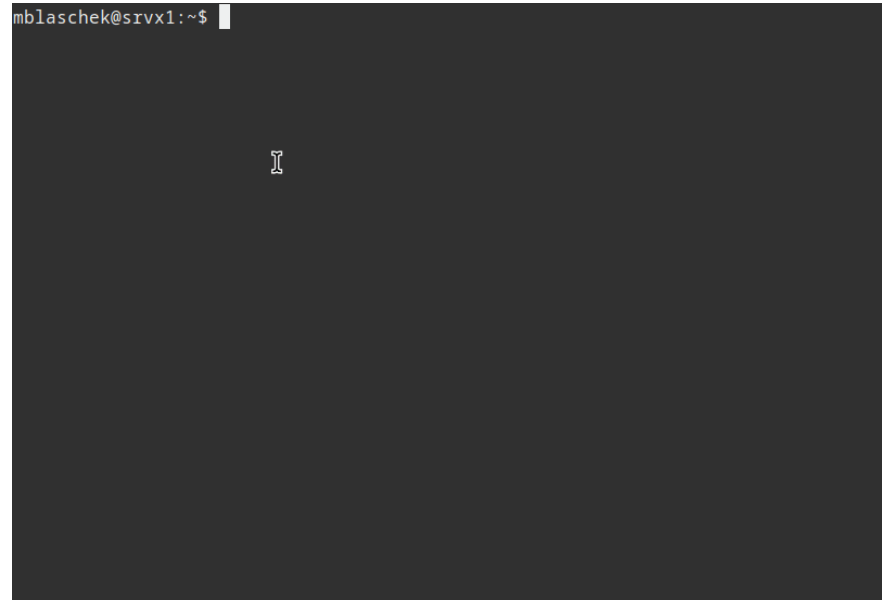
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# Shells & tools – user support

- 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:~$
```

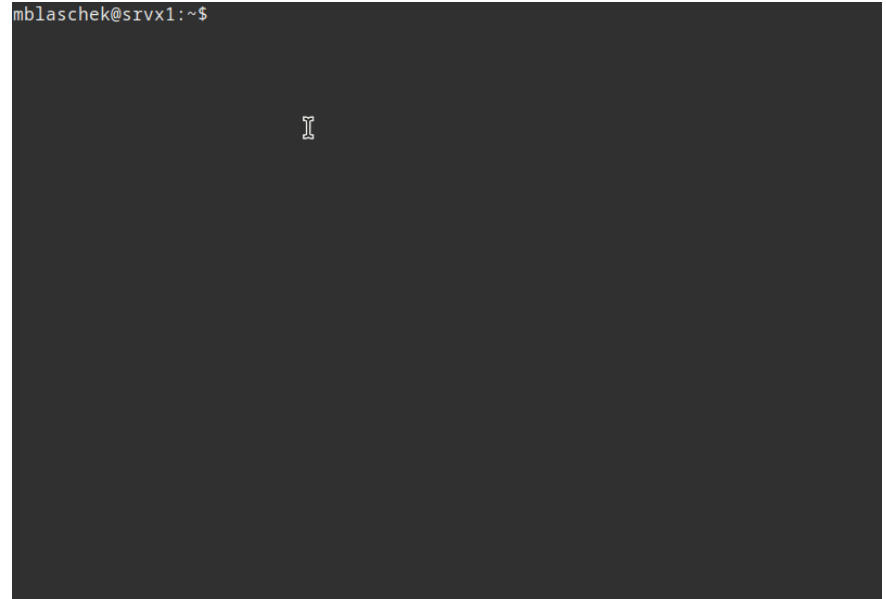
A terminal window with a dark background. The prompt 'mblaschek@srvx1:~\$' is visible at the top left. A white cursor is positioned in the center of the screen.



# Shells & tools – user support

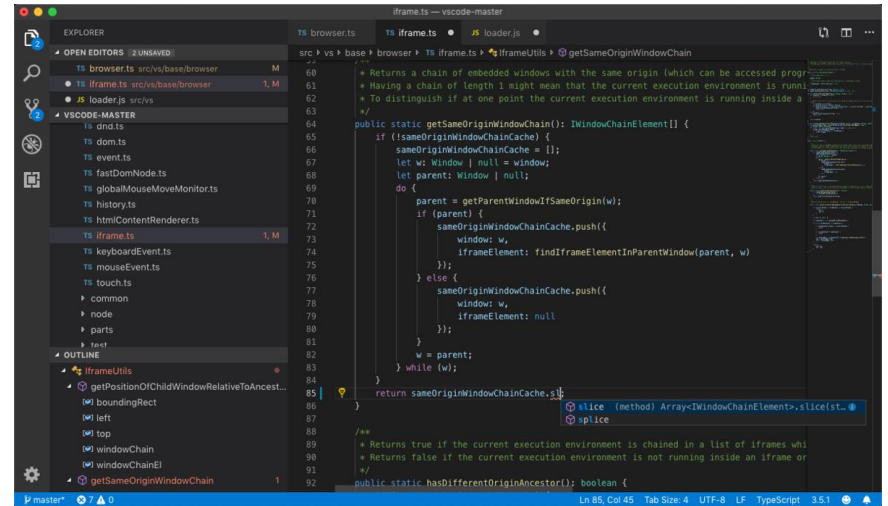
- Most users have bash (`chsh -l`)
- Easy for beginners: `fish`
- Shells use configuration files, e.g. `.bashrc`, `.cshrc`, ...
- Scripts can use all kind of shells
  - `#!/bin/bash`
- Cause of trouble
  - Module load in `.bashrc`, create `alias`  
`mymod="module load <modules>"`

```
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.

# 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



The screenshot shows the VS Code editor interface with a file explorer on the left and a code editor on the right. The file explorer shows a project structure with files like browser.ts, iframe.ts, and loader.ts. The code editor displays the content of 'iframe.ts', which includes a function 'getSameOriginWindowChain' and a utility function 'hasDifferentOriginAncestor'. The code is written in TypeScript and uses recursive logic to traverse a chain of windows. Comments explain the function's purpose: returning a chain of windows with the same origin and distinguishing if the current environment is running inside an iframe.

```
public static getSameOriginWindowChain(): IWindowChainElement[] {
    * 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...
        */
    );
}

/**
 * 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 {
```



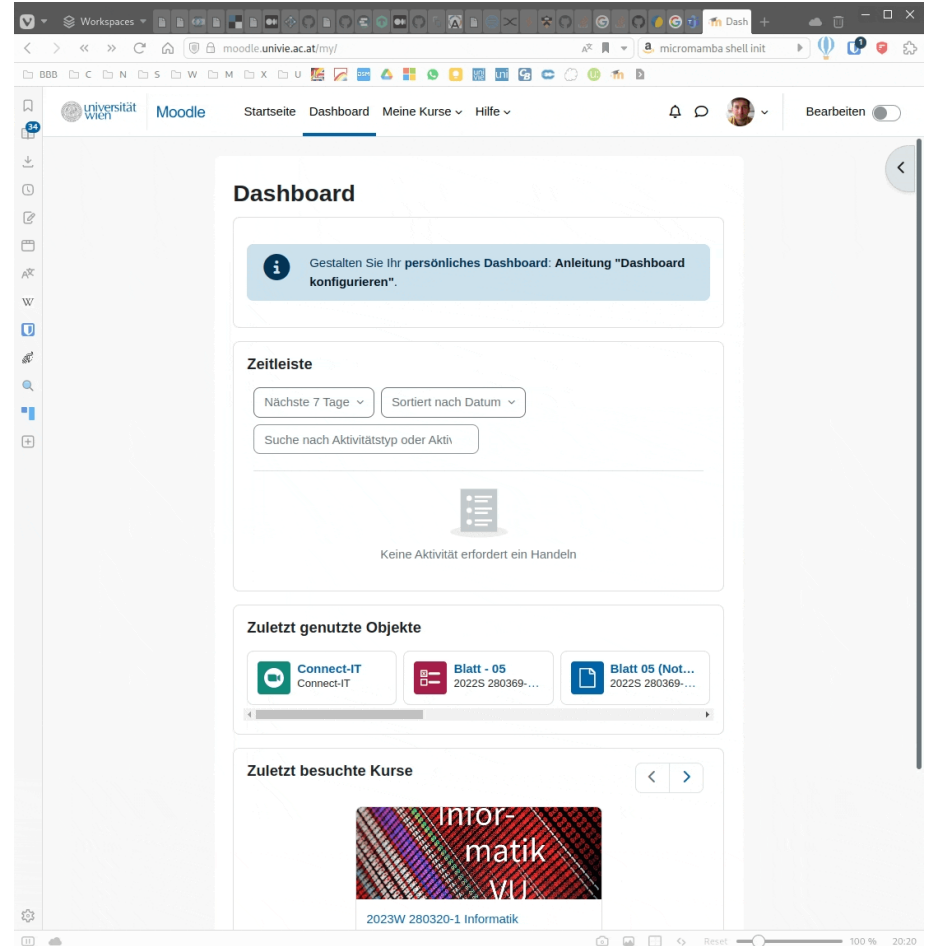
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# clouds and services

@IMG, @ZID, ...

# Clouds and services – Jupyter

- Jupyter Notebook Server (Hub):
  - ~~SRVX1~~ [teachinghub.wolke.img.univie.ac.at](https://teachinghub.wolke.img.univie.ac.at)
    - Soon integrated into jupyter.wolke
  - Teaching + Moodle (login)
  - 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



# Clouds and services – webdata

The screenshot shows a file browser interface for a directory named 'webdata'. The interface includes a sidebar with a tree view of the directory structure, a main table listing files and folders, and a detailed view of the 'webdata' directory.

**webdata** UNIVIE, IMGW Project Fileserver

**webdata**

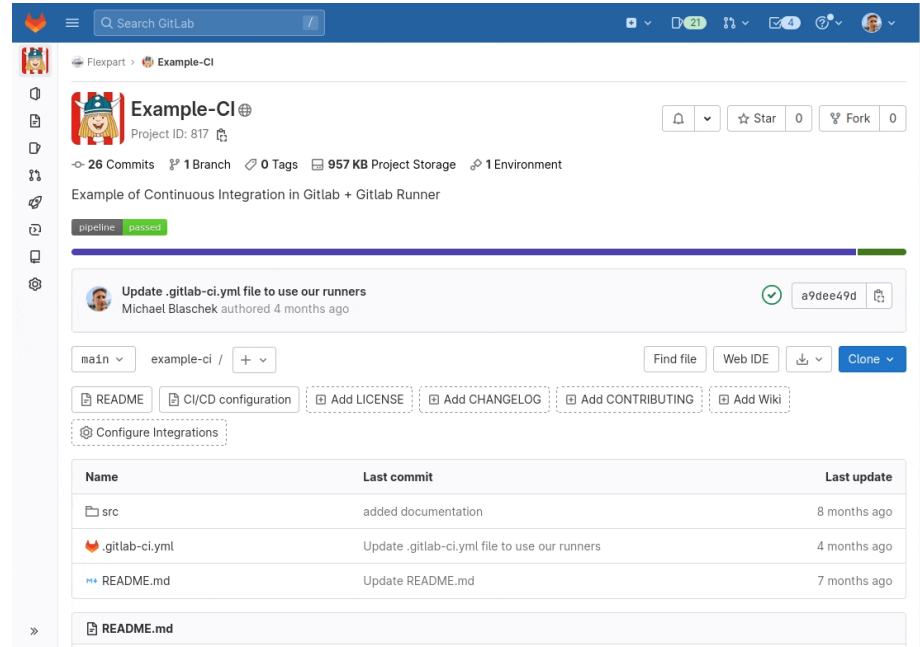
Name	Size
containerlib	
haimberger	
imgw	
kolloquium	
mosaic	
phd-seminar	
scratch	
sonnblick	
TEAMx	
tm-archive	
VERA	
README.md	462 B

**webdata**  
2022-12-16 14:29  
11 folders, 1 files

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

# 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

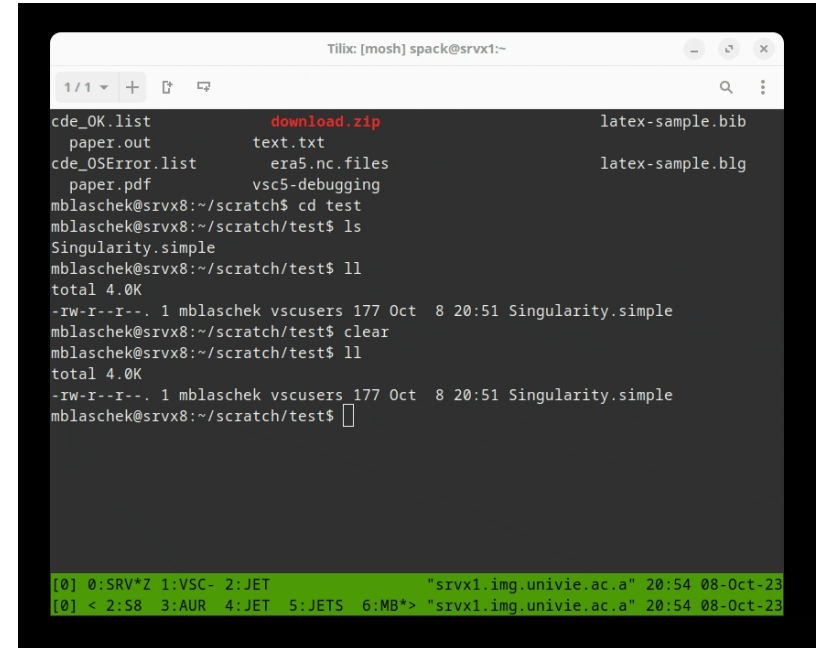


The screenshot shows the GitLab interface for a project named 'Example-CI'. The project is located under the 'Flexpart' group. It has 26 commits, 1 branch, 0 tags, 957 KB of project storage, and 1 environment. The project description is 'Example of Continuous Integration in Gitlab + Gitlab Runner'. A pipeline is shown as 'passed'. A recent commit by Michael Blaschek is titled 'Update .gitlab-ci.yml file to use our runners'. Below the commit, there are buttons for 'Find file', 'Web IDE', 'Download', and 'Clone'. There are also buttons for 'README', 'CI/CD configuration', 'Add LICENSE', 'Add CHANGELOG', 'Add CONTRIBUTING', and 'Add Wiki'. A 'Configure Integrations' button is also present. At the bottom, a table lists the files in the repository:

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



```
Tilix: [mosh] spack@srvx1:~  
1/1 + [?] [?] [?]  
cde_OK.list          download.zip          latex-sample.bib  
  paper.out          text.txt                
cde_05Error.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$
```

```
[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 – Documentation

- Wolke – documentation (computer resources – mkdocs)
- 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 queuing
- VSC4 (5 Nodes)
- VSC5 (11 Nodes)
- Huge development work on
  - SRVX1, AURORA, JET01, JET02
- Long lasting jobs? > queue

## Interaction

---

- Keep your credentials **private**
- **Change** your passwords
- 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!**

## Shared data

---

- `/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

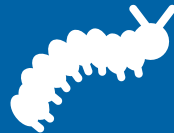
1. Check documentation (*talk to yourself*)
2. Ask a colleague (*talk to another person*)
3. Ask IT (*talk to a group*)

# Contact IT

VSC related? >> Max or Me

Server related? >> Me

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





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# Questions?

PhD seminar

Bare metal, shells and clouds – MB

20.3.2023



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