universität wien

universität wien
Fakultät für Geowissenschaften, Geographie und Astronomie

Bare metal, shells and clouds
IT2Research - UPDATES

14. Oct. 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

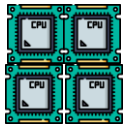
universität wien

Bare metal

Hardware, VSC, ECMWF

Bare metal @ Department – SRVX – JET – VSC Nodes

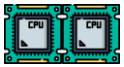
SRVX1



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

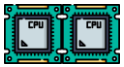
SRVX8

AURORA



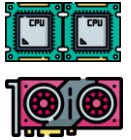
- Arsenal
- 2x CPU
- **Visual Node** (VNC)
- **Development Node**
- Storage Node
  - 800 TB
  - 11 TB SSD

JET



- Arsenal
- 2x Login (hub, vnc)
- **17x** Compute CPU
- **Computing/Post Processing Cluster**
- Storage 3.5 PB Global Storage
- Scheduler (**slurm**)
- Planed: 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 (data, sats, …)👏
- Sign up free.

ECMWF

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

eodc

- Jupyter - eodc.wolke.img.univie.ac.at
- EODC – products (Sentinel, GPSRO, ERA5,…)

Leonardo

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

LUMI

universität wien

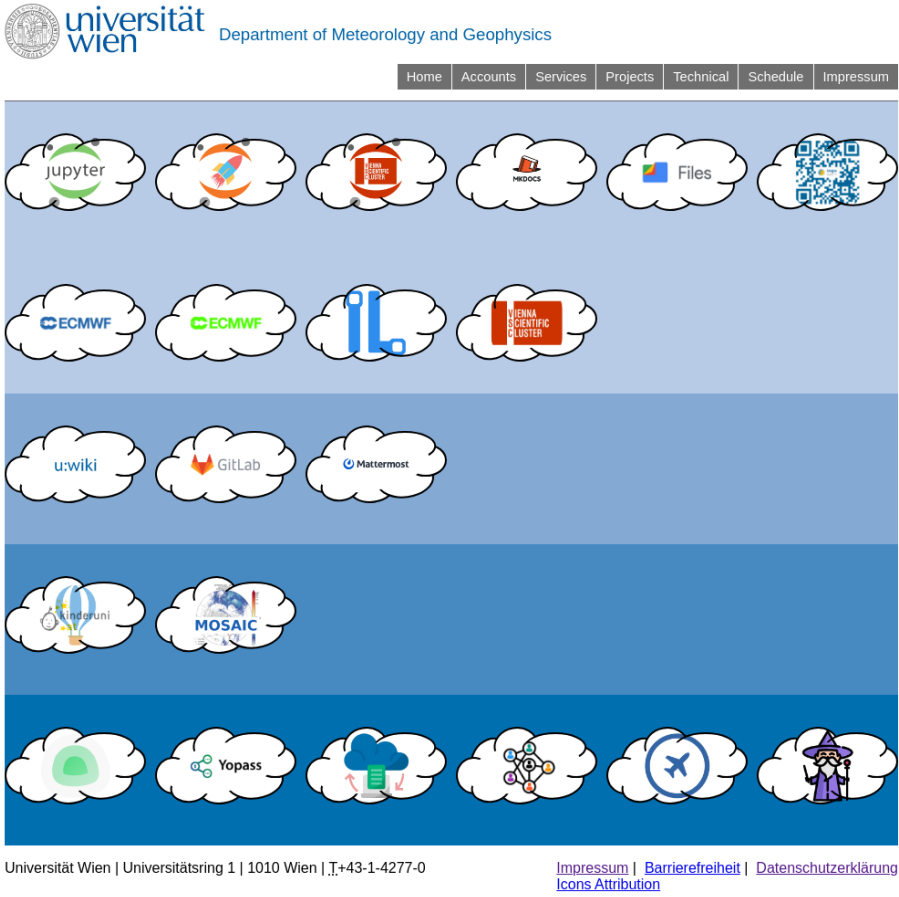
Shells & tools

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

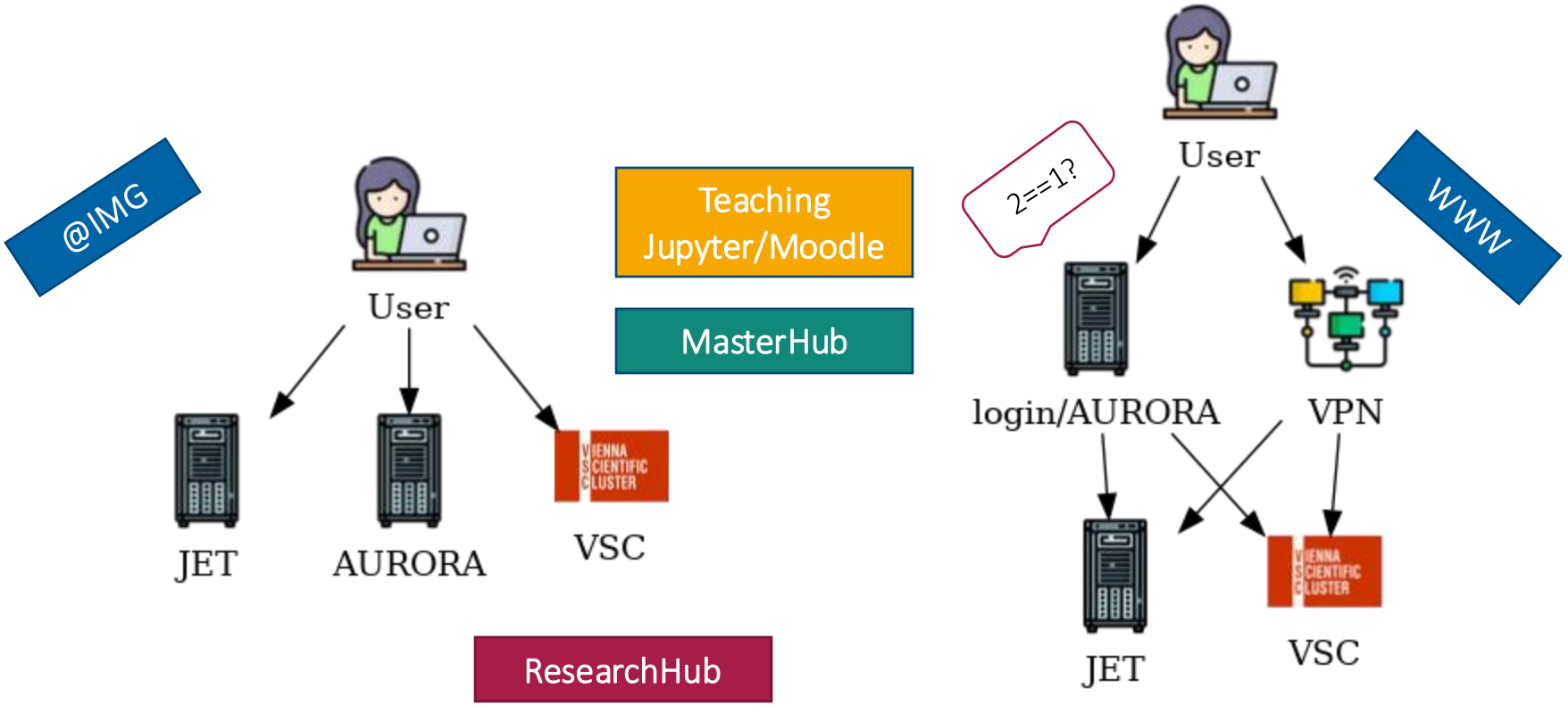
Questions?
Are you missing something?



universität wien

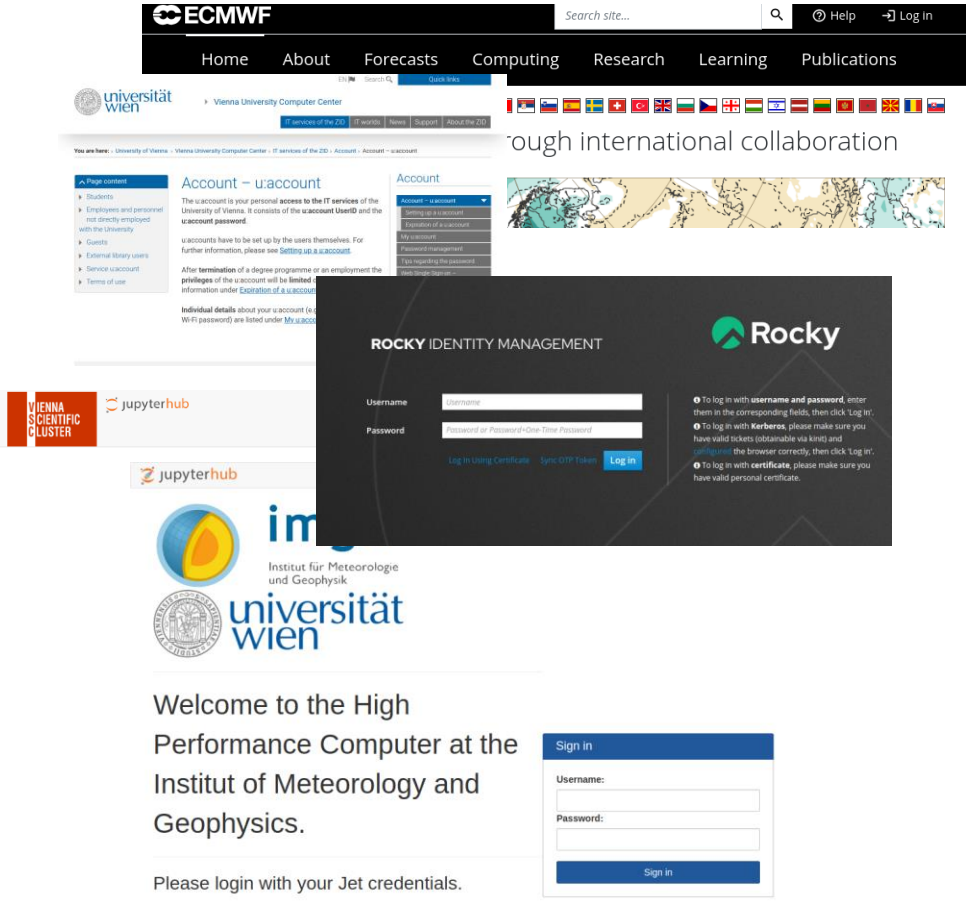
imgw
Institut für Meteorologie und Geophysik

Shells & tools – Access



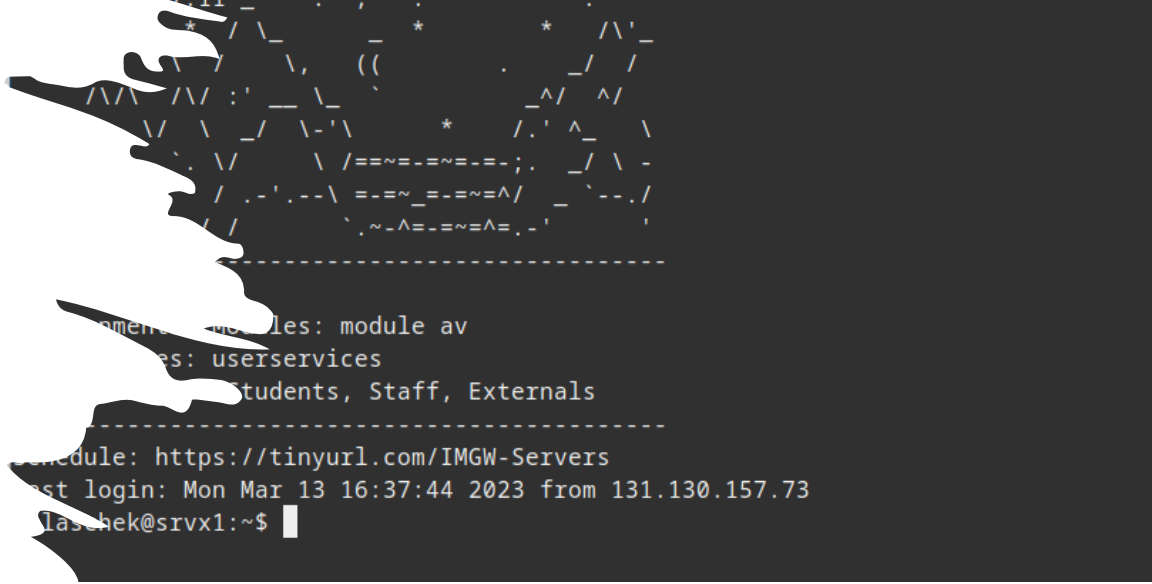
Shells & tools – Accounts

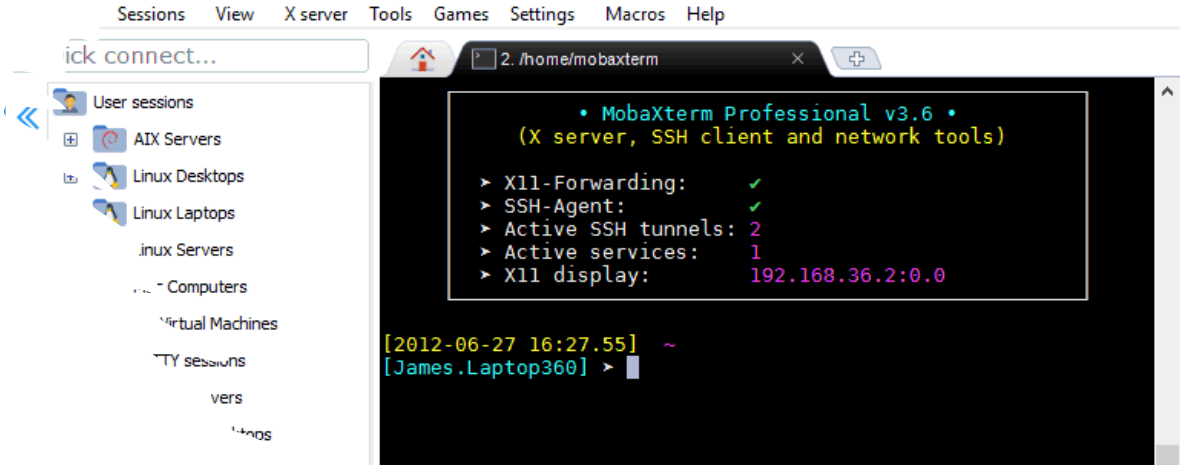
1. **u:account**
   - All ZID services
   - Jupyterhub @Moodle
2. **w:account** (Wolke IMG account)
   - All servers
   - Jupyterhub on JET
3. ~~**t:account** TeachingHub~~
4. **ec:account** (ECMWF)
5. **vsc:account** (VSC)



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
  - `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

universität wien

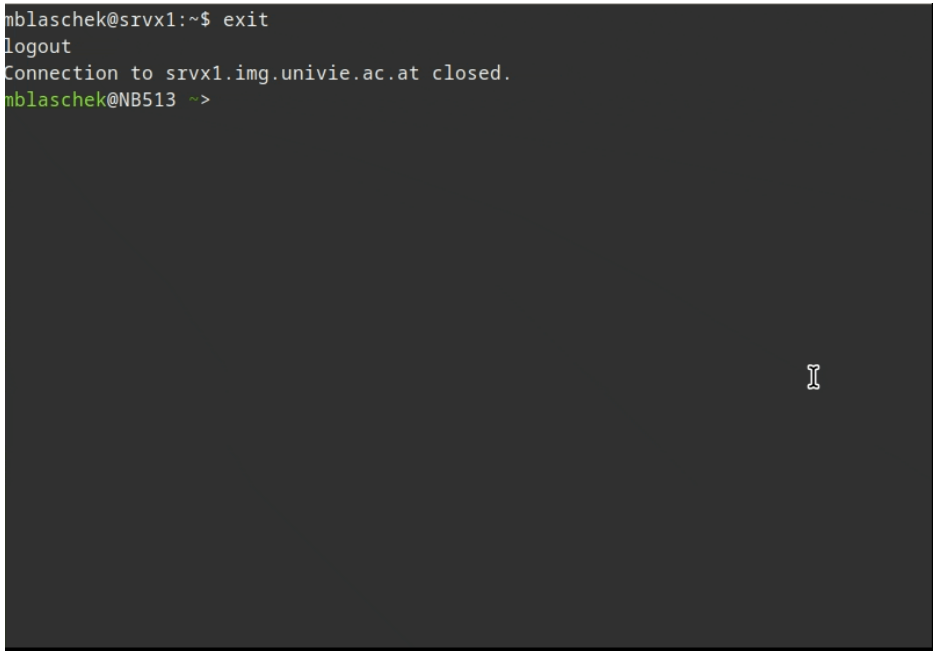
Shells & tools – userservices filesender

- `userservices` – collection of useful scripts
  - `filesender` – ACOnet 250 GB
  - `quota` – storage quota of user
  - `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 ~~sshtools~~

- `userservices` – collection of useful scripts
  - `fi` … 250 GB
  - `qu` … er
  - ~~`ss` … ager~~
  - `transfersh` – send small files (<500 MB)
  - `ucloud` – upload to u:cloud
  - `yopass` – encrypt messages
  - `vnc` – Virtual desktop on SRVX8
  - `weather` – current weather info

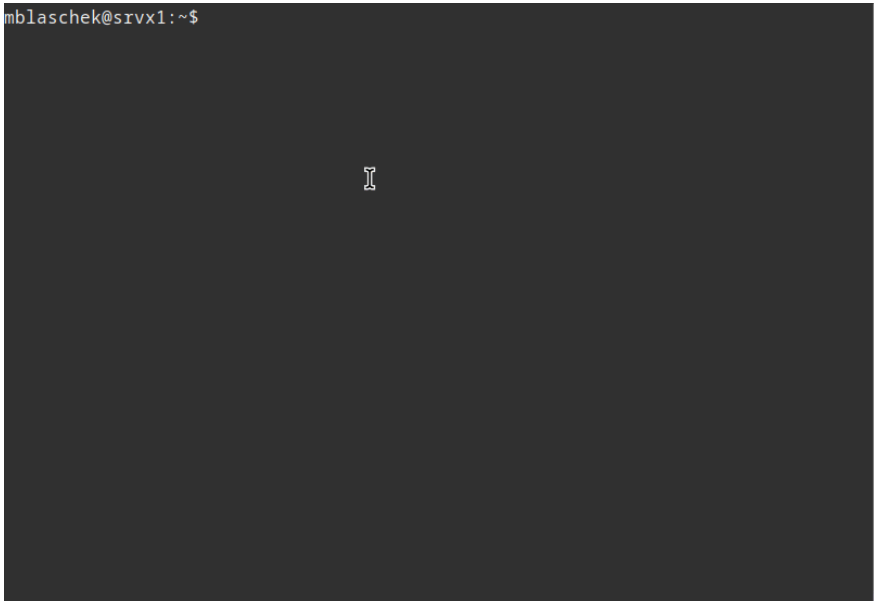
Has been replaced and is available now all the time



universität wien

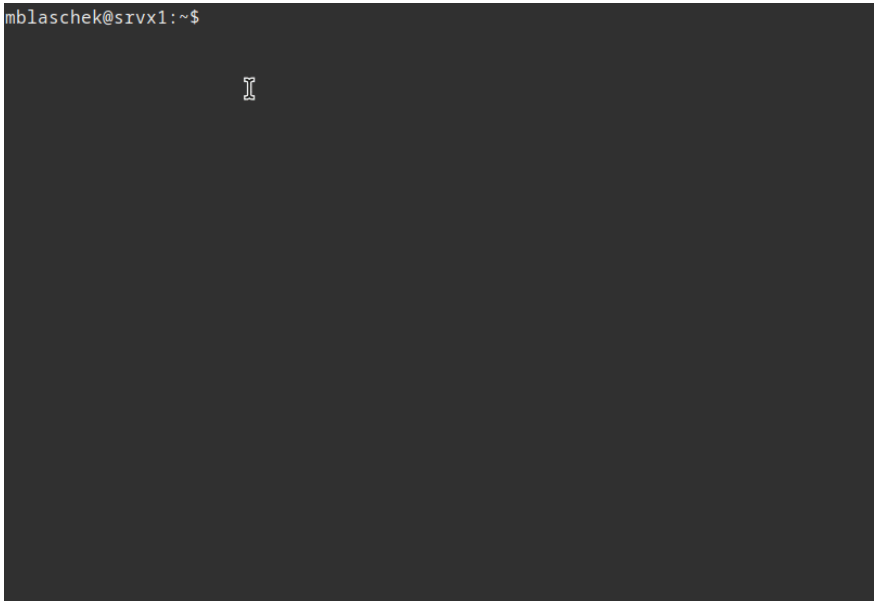
Shells & tools – userservices transfersh

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



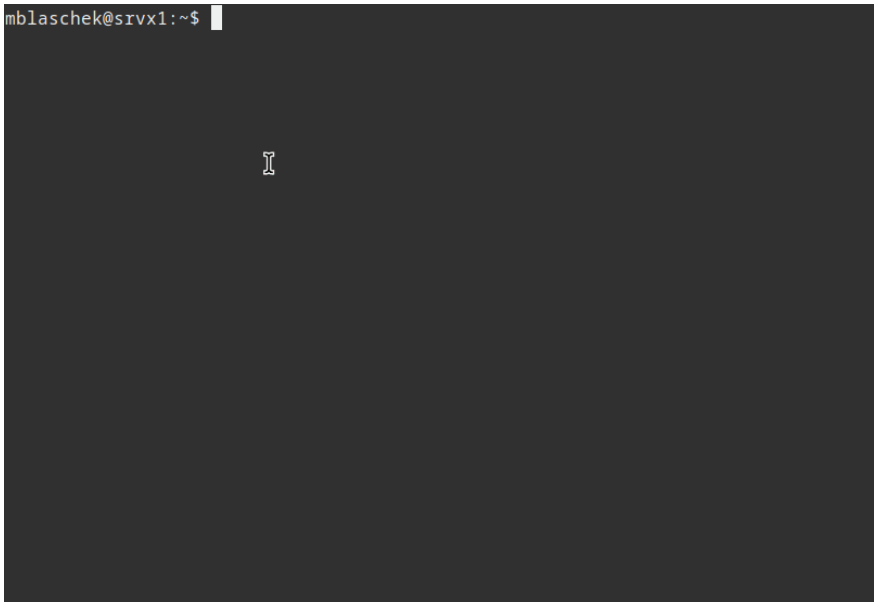
Shells & tools – userservices vnc (JET01, AURORA)

- `userservices` – collection of useful scripts
  - `filesender` – ACOnet 250 GB
  - `quota` – storage quota of user
  - `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 – 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`

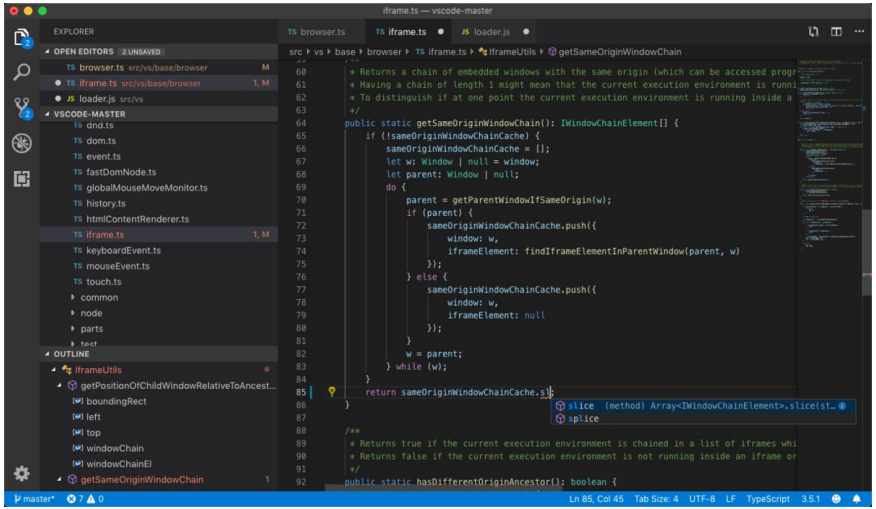


Shells & tools – user support

- 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>"`

Shells & tools – user support - recommendations

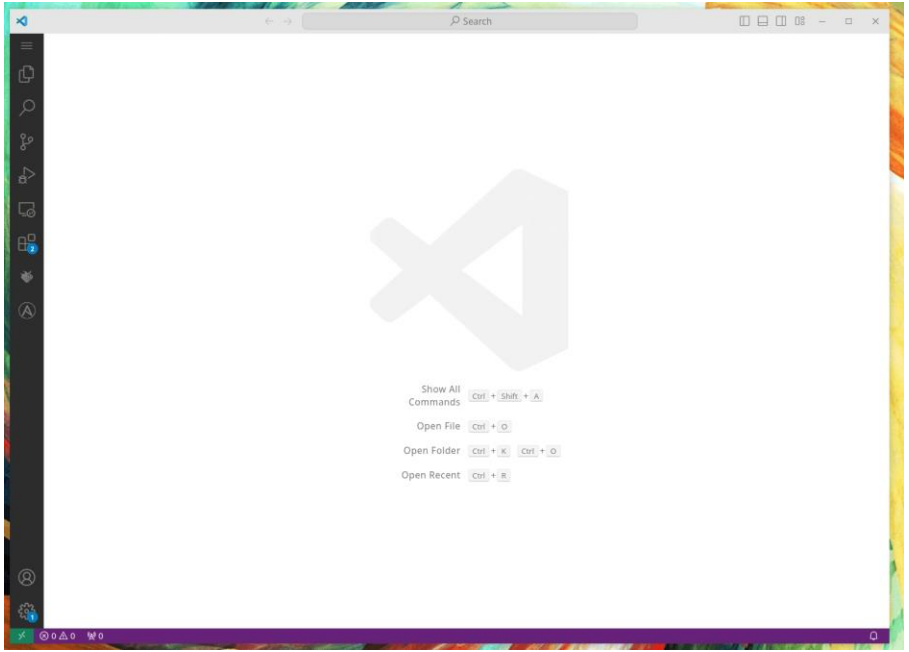
- Editors: **vim**, nano
- Dev Environment: **VSCode**, Code OSS
  - Extensions: Remote SSH, Dev Containers, Python, Notebooks, Modern Fortran, …
  - Git fully integrated
- Python: build your own environment
  - Use conda or **micromamba**
  - Install packages, create environment file for a working environment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



universität wien

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)

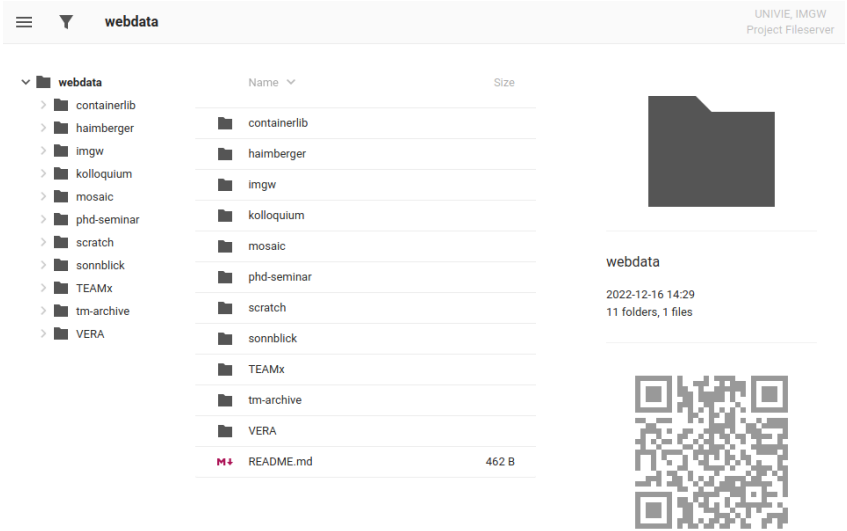


universität wien

clouds and services

@IMG, @ZID, ...

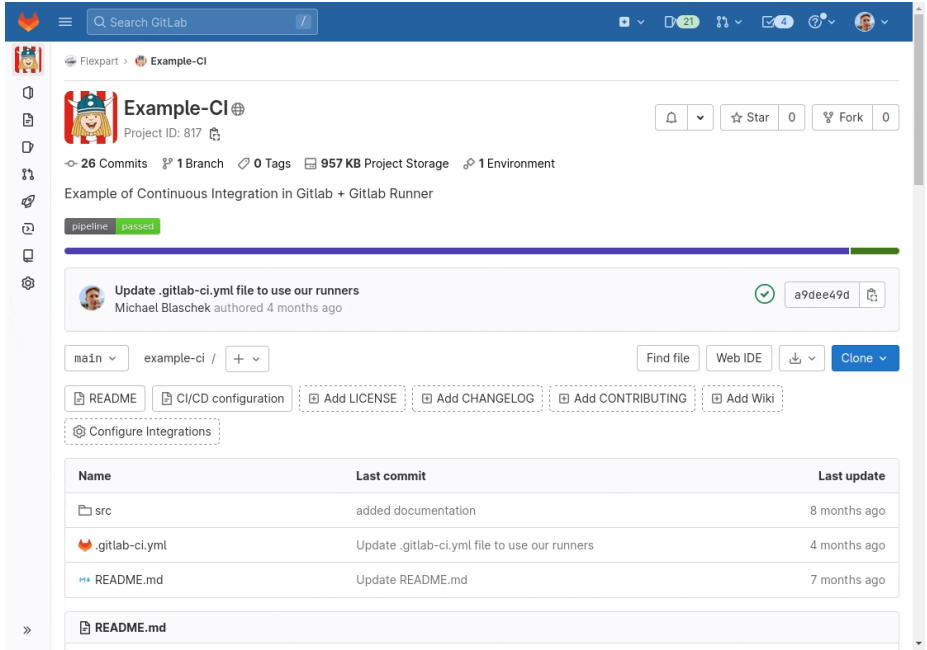
Clouds and services – webdata



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

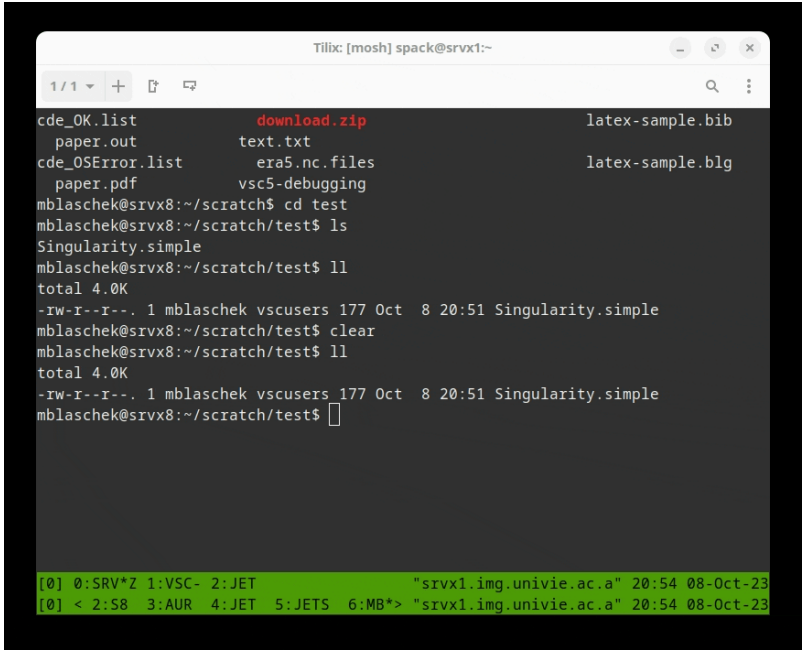
Clouds and services – gitlab

- Continuous integration (CI) and development
  - Code testing
  - Deployment
  - Development in groups
- 4 Runners (IMGW, Flexpart, Climate, DA)
- Example: https://gitlab.phaidra.org/imgw/example-ci



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 (request subuid)
- Integrate with gitlab-ci
- Publish on IMGW registry: harbor.wolke.img.univie.ac.at
  - Access from IMGW network, otherwise need a secret password.



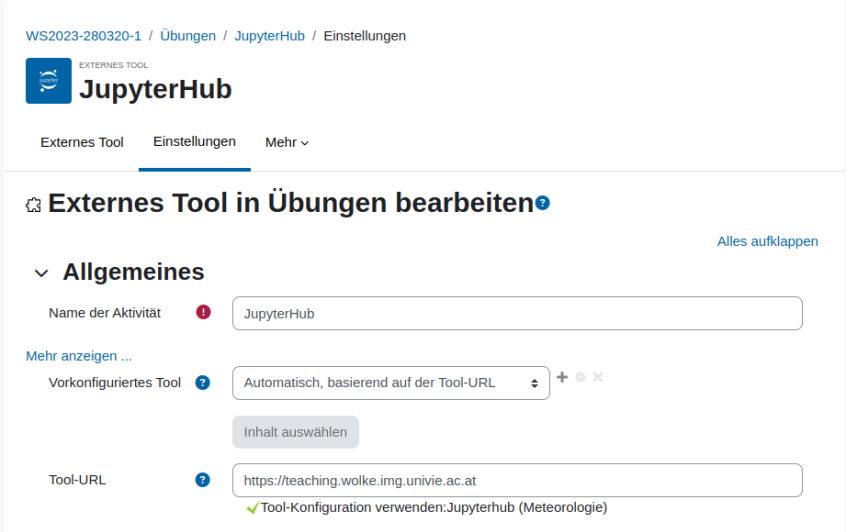
Clouds and services – ZID

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

Resources @IMG

Resources – Teaching

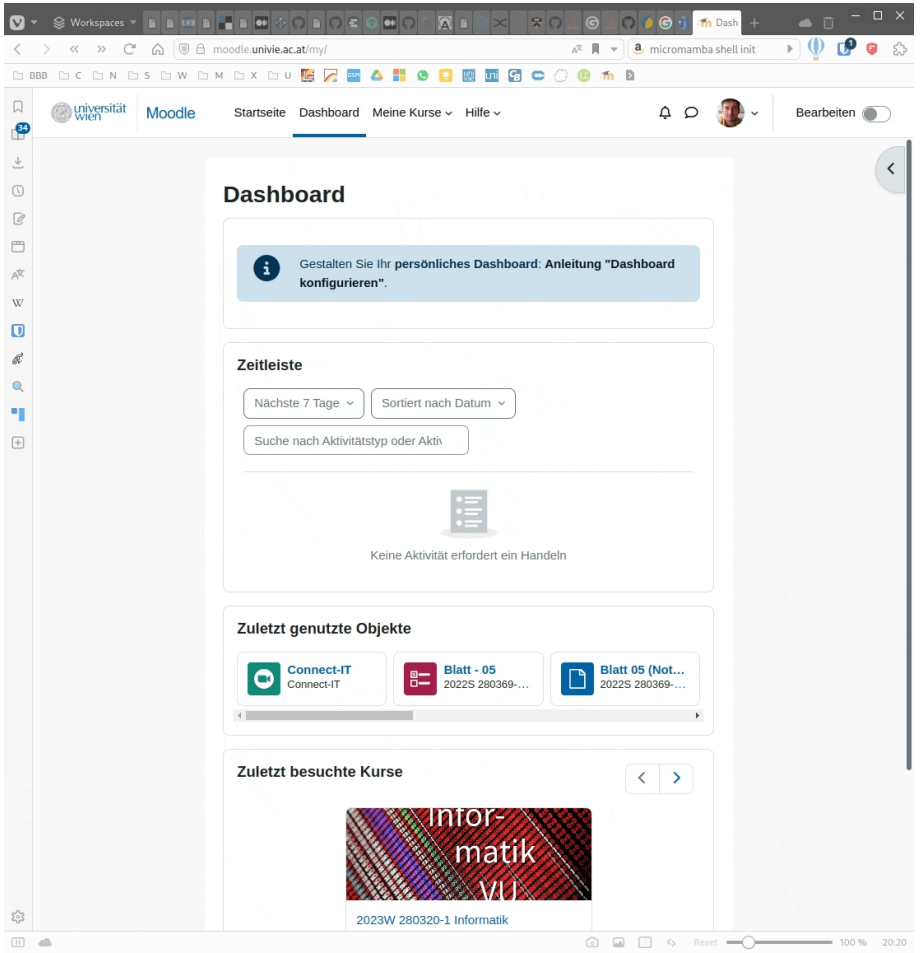
- Lots of information in u:wiki – Tutorials – Teaching
- Moodle (u:account)
- **TeachingHubv2** for your course
- Student Response System (SRS)
  - srs.univie.ac.at (feedback, questions, live)



universität wien

Resources – Jupyter

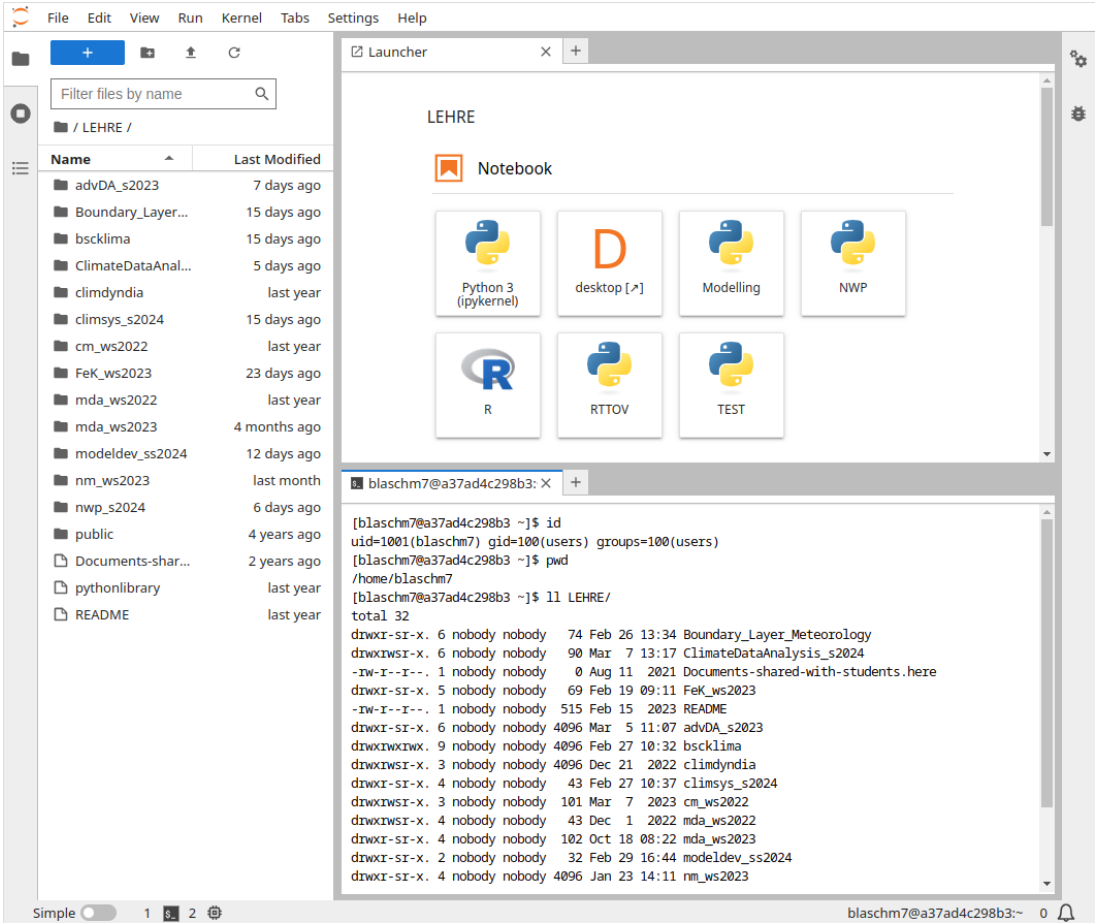
- Jupyter Notebook Server (Hub):
  - Teaching + Moodle (login)
    - Only SPL28, request for other courses
  - MASTER quell.wolke.img.univie.ac.at
  - JET jupyter.wolke.img.univie.ac.at
  - VSC Hub jupyterhub.vsc.ac.at
  - WEkEO wekeo.eu
  - EODC eodc.wolke.img.univie.ac.at
- Kernels with different python versions, packages
- Notebooks - Documentation + Code



universität wien

Working with the Moodle Jupyter Hub (TEACHING 👩🏼‍🎓)

- All SPL28 students/lecturers have access
- **$HOME/LEHRE** maps to **/srvfs/lehre**
- **Quota**: 20 GB, 100k files ❓
- IMGW user **!=** teaching hub user
- Transfer files (**scp**, download) or userservices transfersh [file] + wget
- **Purge every September (**how to communicate to users?**)**



universität wien

Resources – Software

- I vote for open source software
- But UNIVIE offers software for staff
  - SAM – sam.univie.ac.at/wm
  - Self service (user: `u\[u:account]`)
  - MS365, Adobe, Labview, Matlab,…
  - Search Catalog (look for unmanaged)
  - Ask Supervisor first if that is ok.
  - Request, Sends email to IT (need to approve)

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

universität wien

Resources – People

- **You can ask people to help you (no shame)**
- e.g.
  - IT – Michael Blaschek (HPC, Python, CI, Fortran, …)
- Experts
  - Leopold Haimberger (Python, Fortran, …)
  - Stefano Serafin (WRF, Python, Post processing,...)
  - Marina Dütsch (Fortran, Python, 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

universität wien

rules

Really ???

universität wien

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
  - AURORA, JET01, JET02
- Long lasting jobs? > queue

Interaction

- 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**

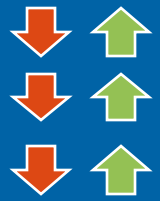
Shared data

- `/srvfs/data`
- `/srvfs/shared`
- `/jetfs/shared-data`
- **Respect other users**
- **Write a documentation**
- Give access to groups (met-…,geo-…)
- JET is shared on VSC
  - `/gpfs/jetfs`
  - **`Permissions!!!!!`**

universität wien

Communication is keen

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



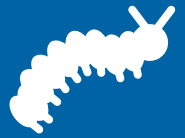
universität wien

Contact IT

VSC related? >> Me

Server related? >> Me

Everything else/safe option >> it.img-wien@univie.ac.at or **mattermost – bugs**



universität wien

universität wien

Questions?

PhD seminar

Bare metal, shells and clouds – MB

On the wiki:
tutorials – Computing