Bare metal, shells and clouds IT2Research

9. Oktober 2023

M. Blaschek

PhD Seminar @ IMG Vienna

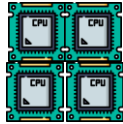# What you can expect from this presentation

Bare metal

Hardware, VSC, ECMWF

Bare metal @ Department – SRVX – JET – VSC Nodes

SRVX1
- Arsenal
- 4x CPU
- Development Node
- **Teaching Node**
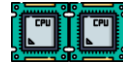- Storage Node
  - 400 TB (users)
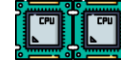 - 400 TB (scratch)

SRVX8

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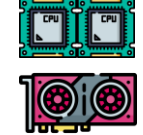- 2x CPU
- **Visual Node** (VNC)
- **Development Node**

JET
- Arsenal
- 2x Login
- 7x Compute CPU
- **Computing/Post Processing Cluster**
- Storage 3.5 PB Global Storage
- Scheduler (**slurm**)
- Planed: 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
- EODC – products (Sentinel, GPSRO, ERA5,…)

Leonardo

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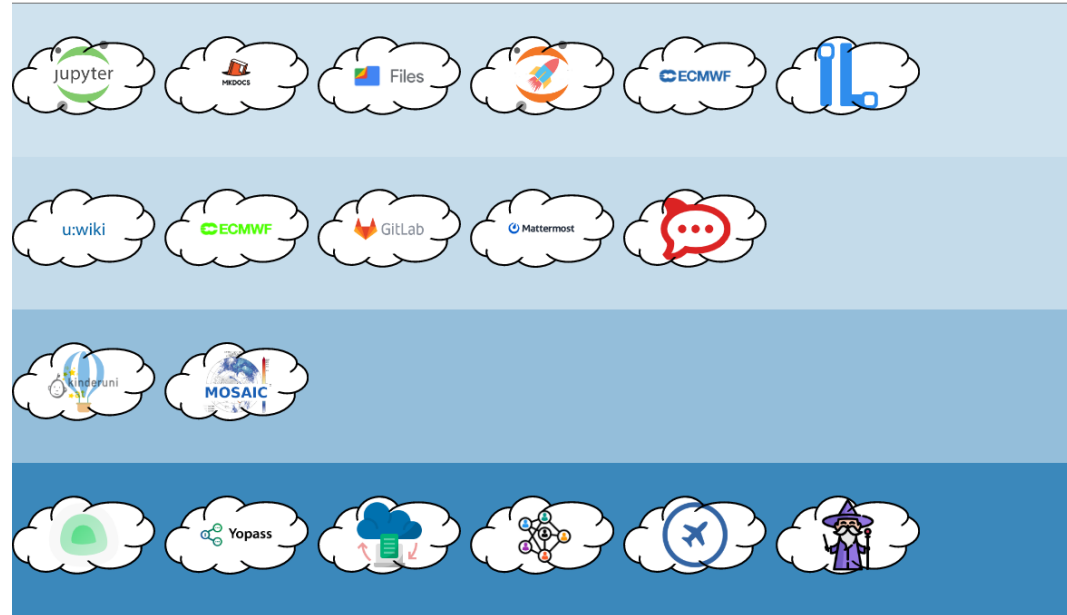
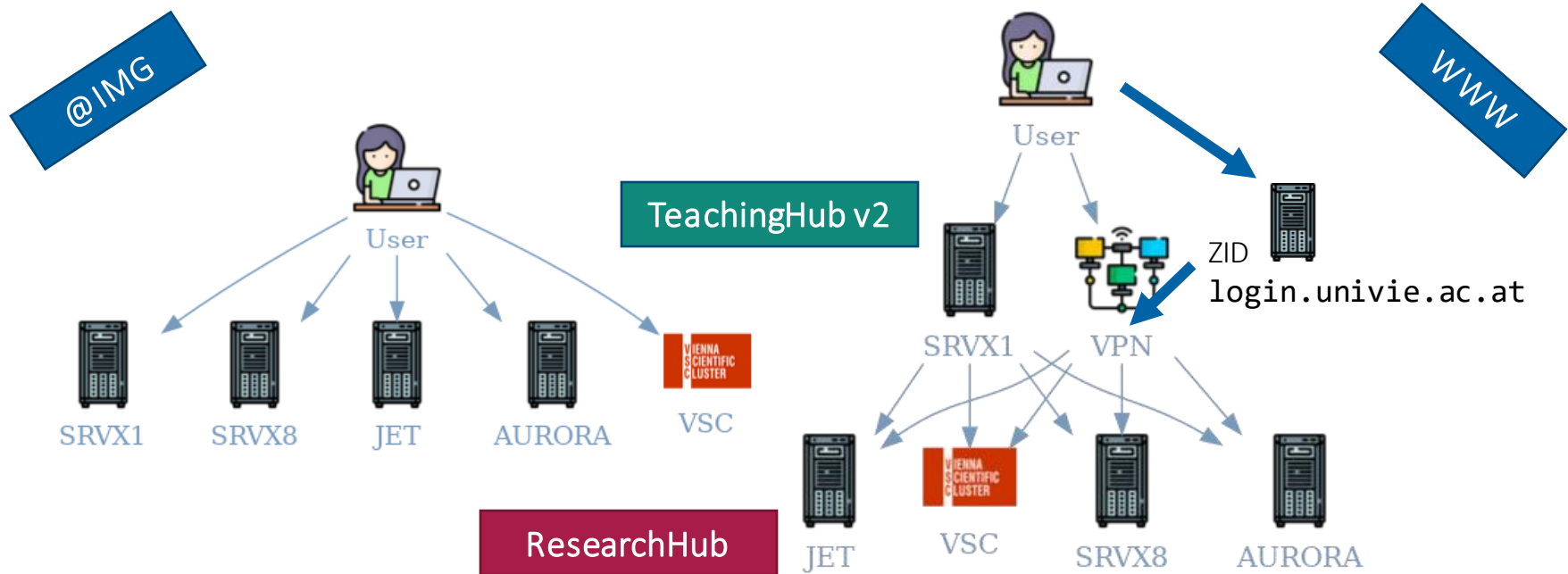universität wien

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

Shells & tools – Access

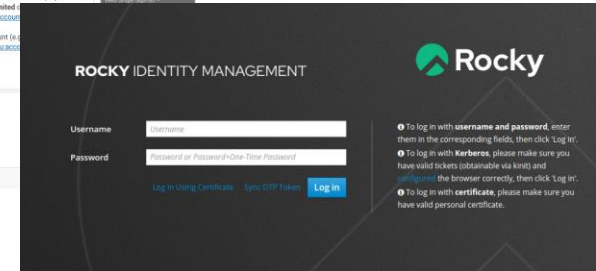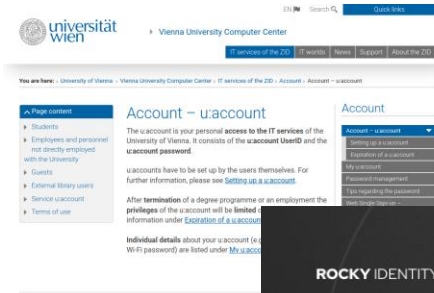# Shells & tools – Accounts

1. **u:account**

   - All ZID services

   - Jupyterhub @Moodle

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

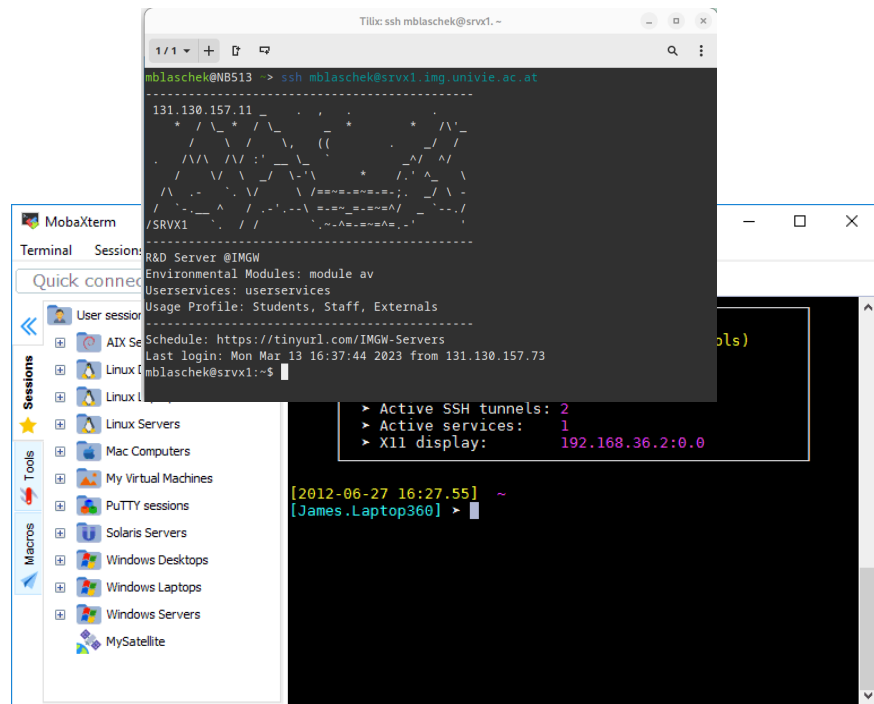   - All servers

   - 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)

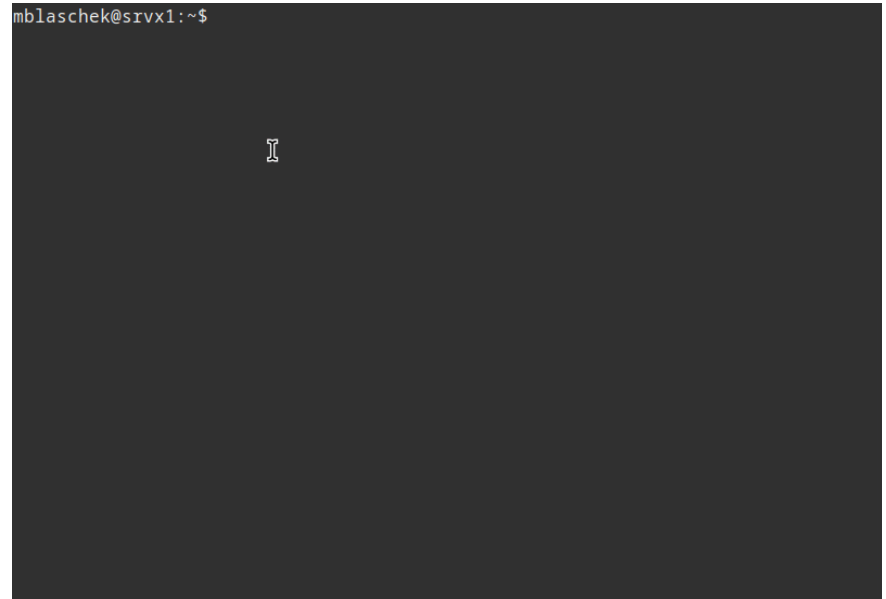universität wien
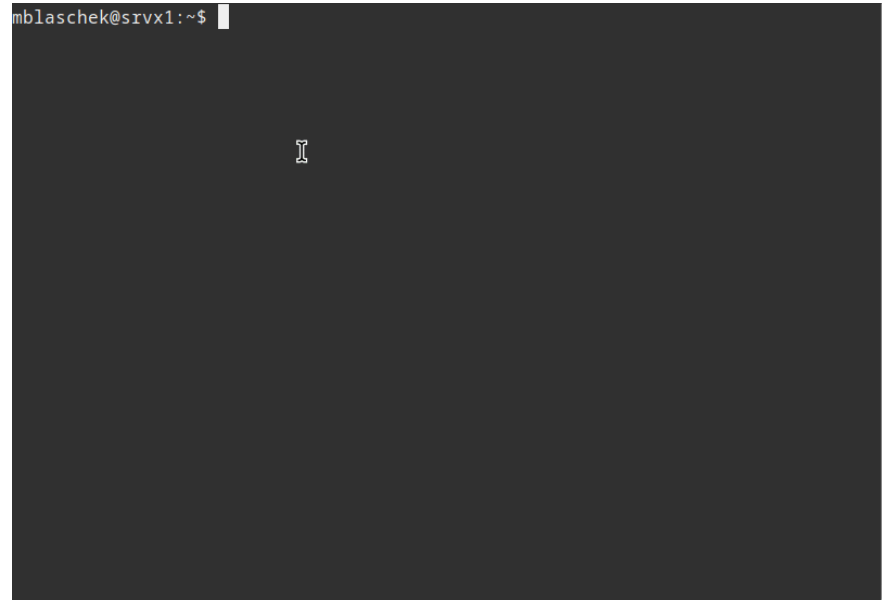
Shells & tools – userservices

- **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

```
mblaschek@NB513 ~>
```

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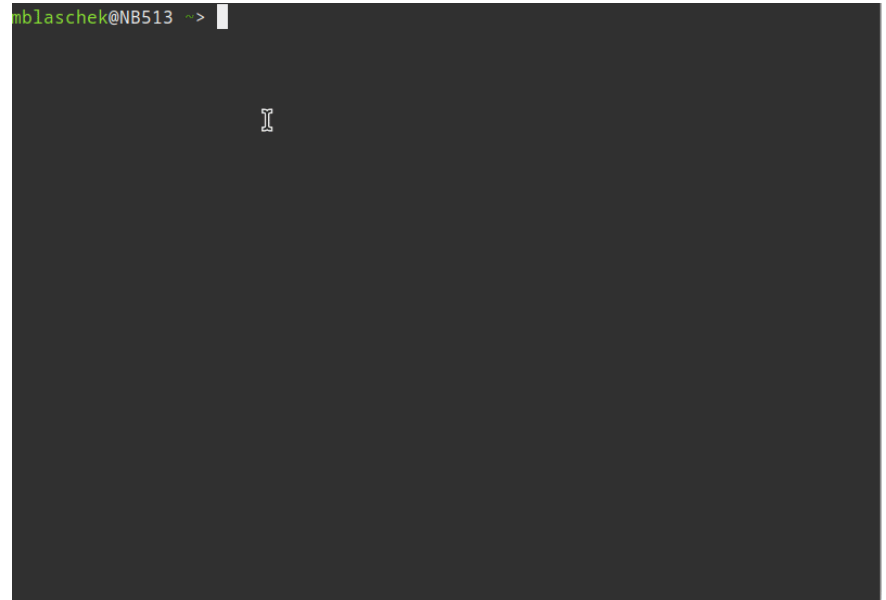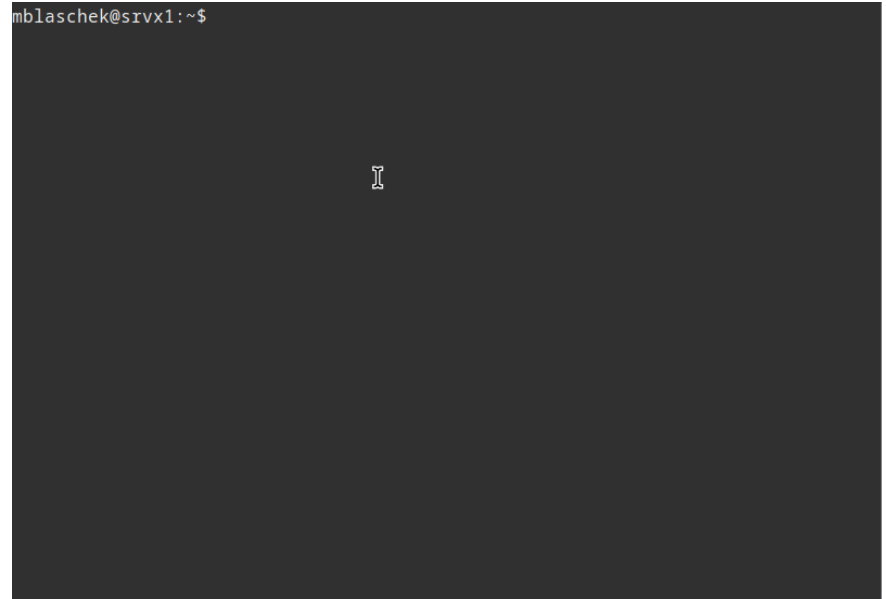
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mblaschek@srvx1:~$
```

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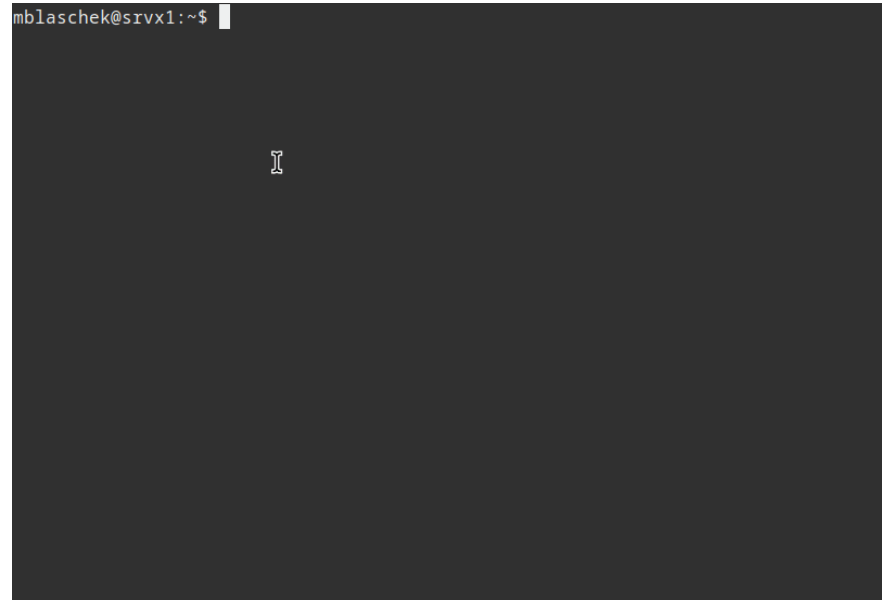wien

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Shells & tools – userservices vnc

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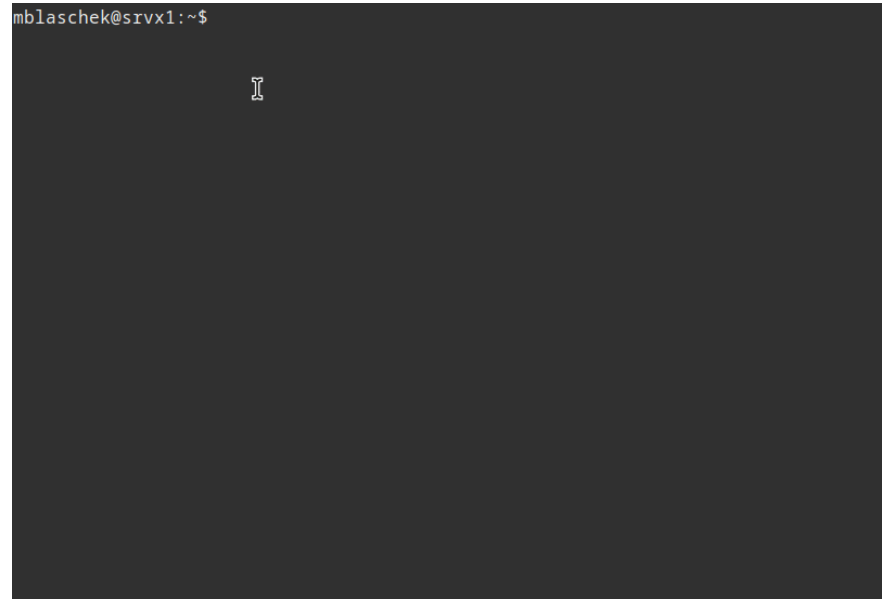
Shells & tools – user support

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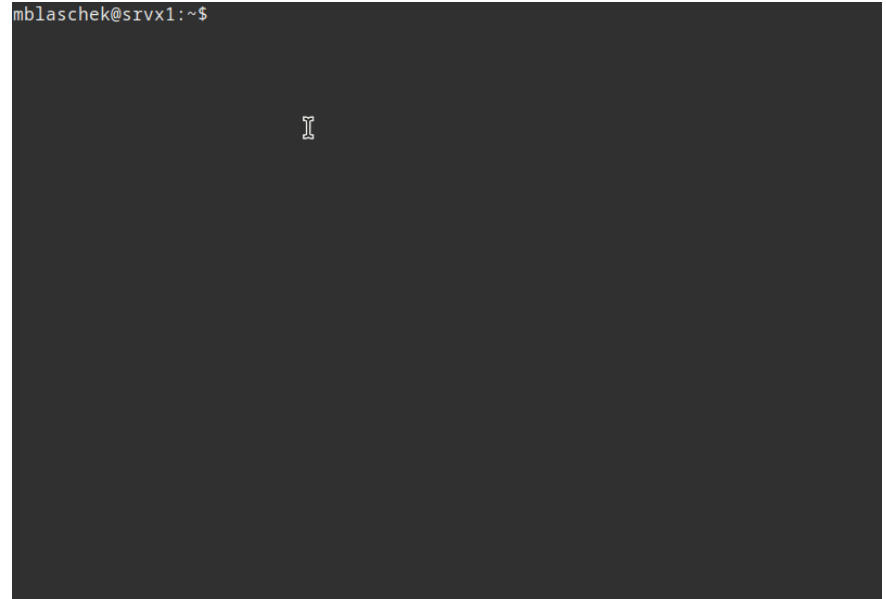
Shells & tools – user support
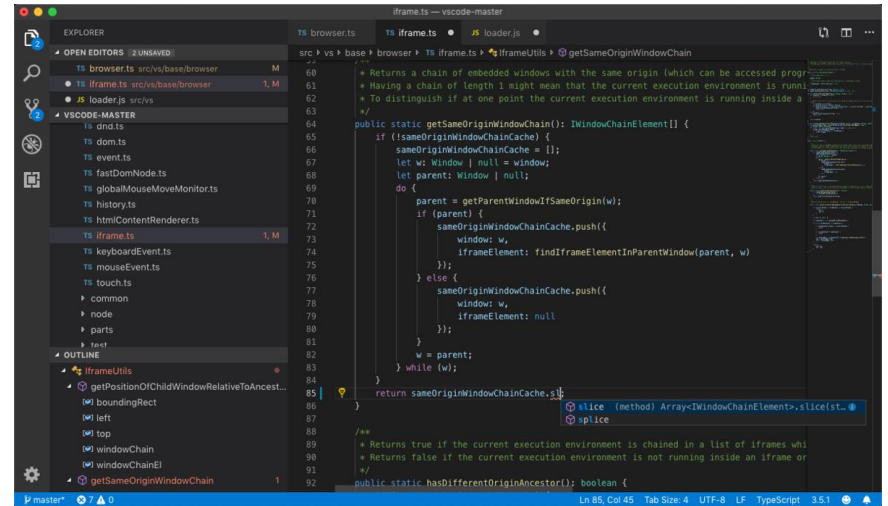
- Most users have bash (`chsh -l`)
- Easy for beginners: `fish`
- Shells use configuration files, e.g. `.bashrc, .cshrc, ...`
- Scripts can use all kind of shells
  - `#!/bin/bash`
- Cause of trouble
  - Module load in `.bashrc`, create `alias mymod="module load <modules>"`

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

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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)
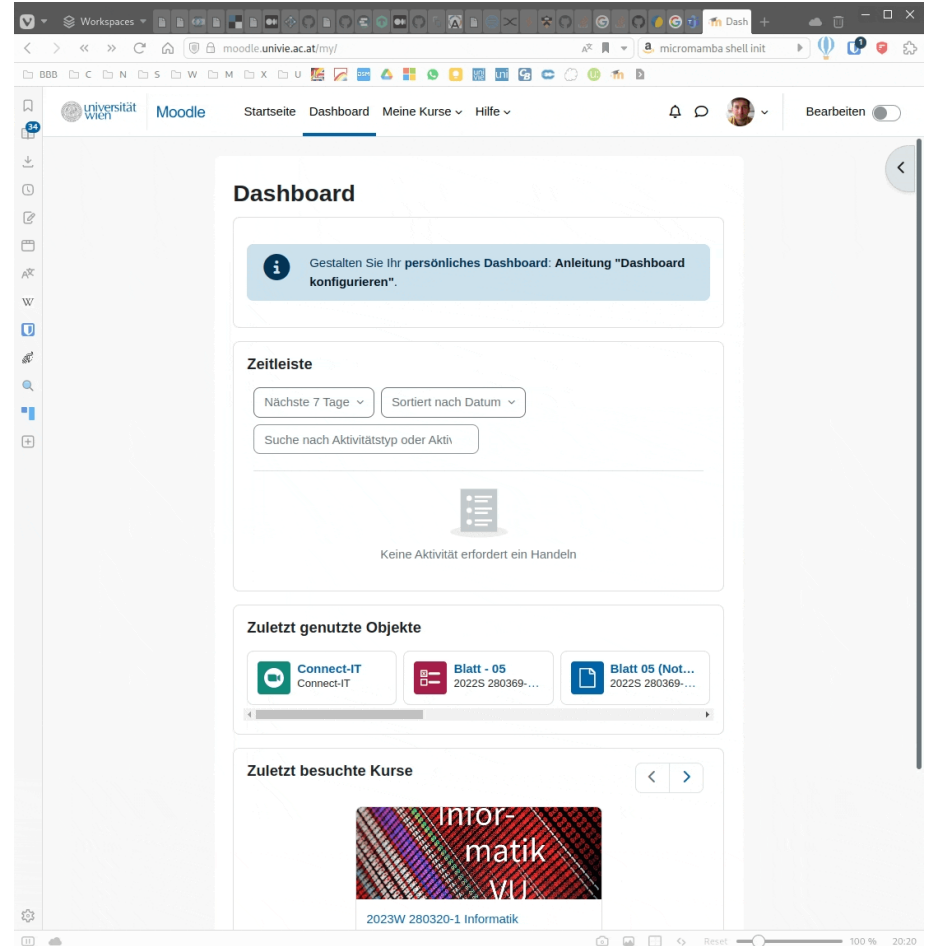 - Add as a kernel to TeachingHub/ResearchHub

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clouds and services

@IMG, @ZID, …

Clouds and services – Jupyter

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

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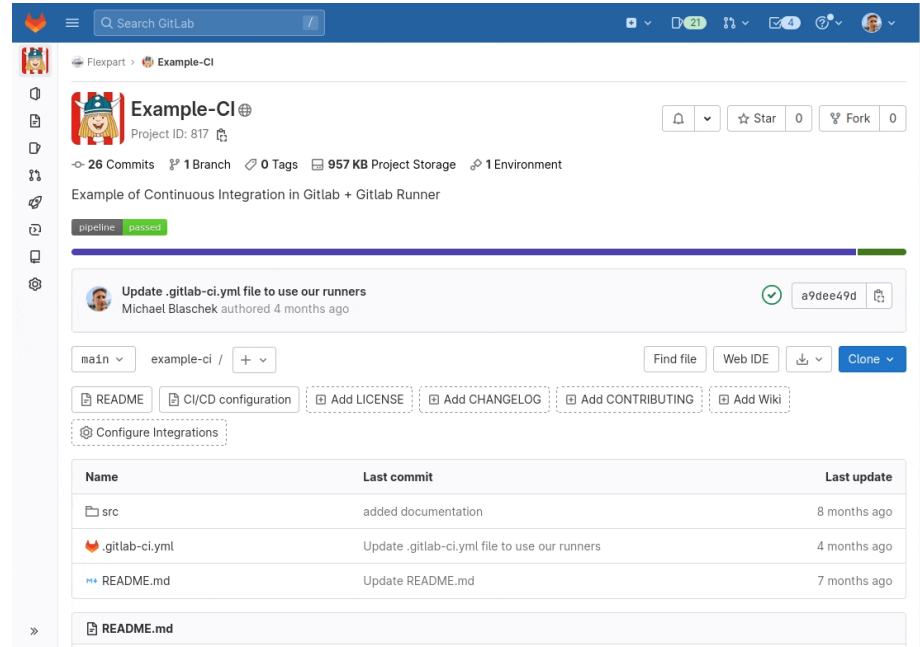
- Wolke > files
- `/mnt/scratch/webdata`
- Request a directory or create one in scratch
- Authentication can be requested too user:pwd
- Accessible to everybody

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

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
- experimental

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, …

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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)

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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 (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

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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 ???

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`

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Communication is keen
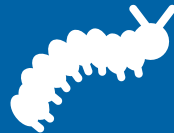
1. Check documentation (*talk to yourself*)

2. Ask a colleague (*talk to another person*)

3. Ask IT (*talk to a group*)

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Contact IT

VSC related? >> Max or Me

Server related? >> Me

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

Questions?

PhD seminar

Bare metal, shells and clouds – MB

20.3.2023