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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



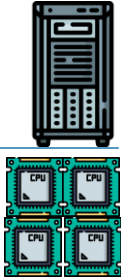
 Bare metal

Hardware, VSC, ECMWF

Bare metal @ Department – SRVX – JET – VSC Nodes

SRVX1

- Arsenal
- 4x CPU
- Teaching Node

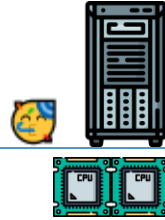


SRVX8



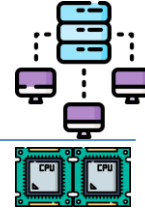
AURORA

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



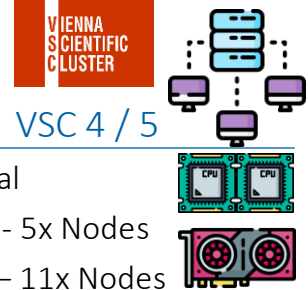
JET

- 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



- 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**.



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



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



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





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

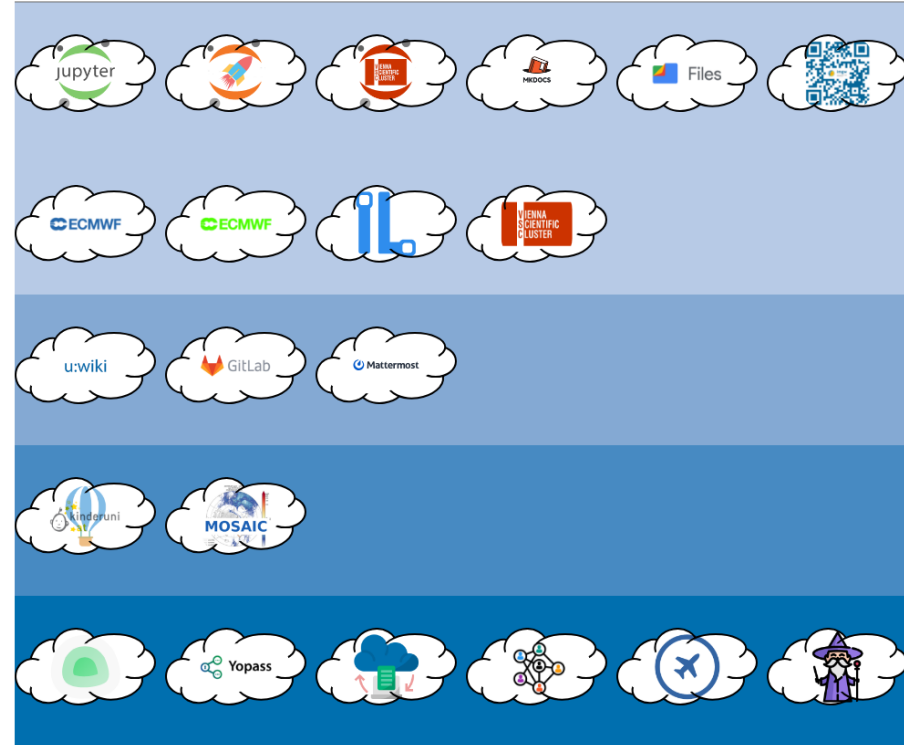
Questions?
Are you missing
something?



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Department of Meteorology and Geophysics

Home Accounts Services Projects Technical Schedule Impressum



Universität Wien | Universitätsring 1 | 1010 Wien | T.+43-1-4277-0

[Impressum](#) | [Barrierefreiheit](#) | [Datenschutzerklärung](#)
[Icons Attribution](#)

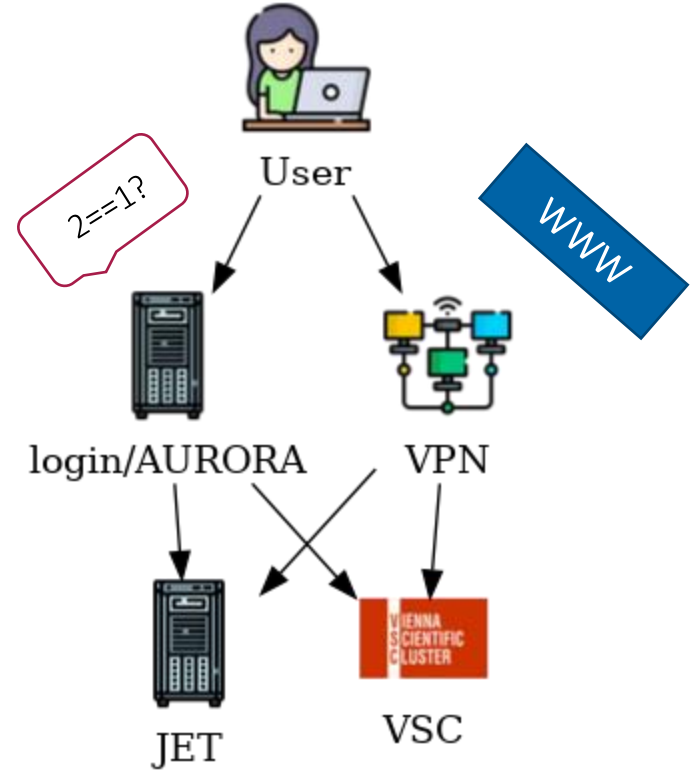
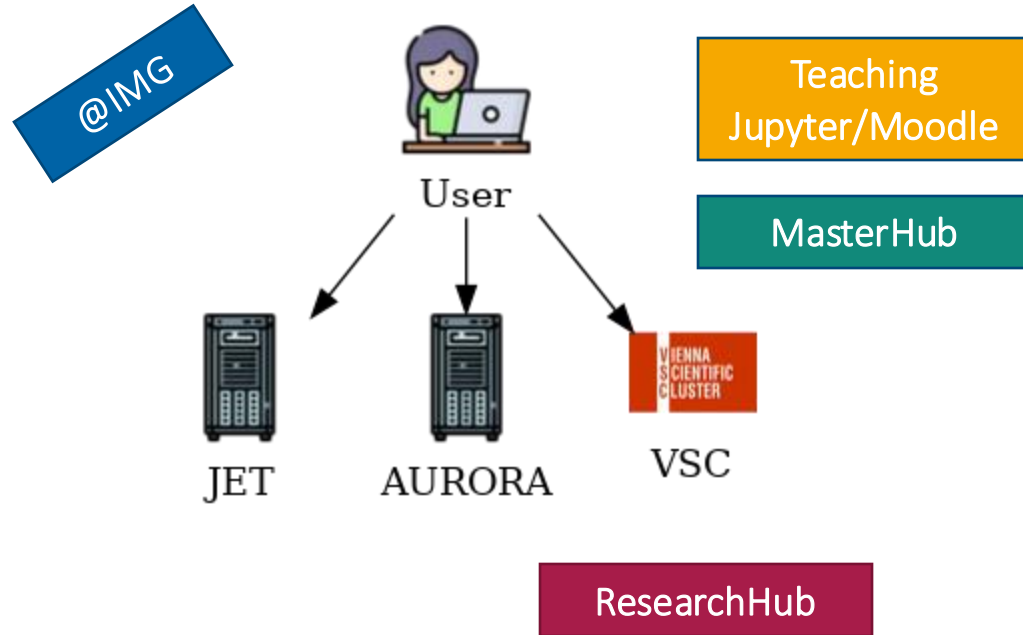


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und Geophysik

Shells & tools – Access



Shells & tools – Accounts

1. u:account

- All ZID services
- Jupyterhub @Moodle

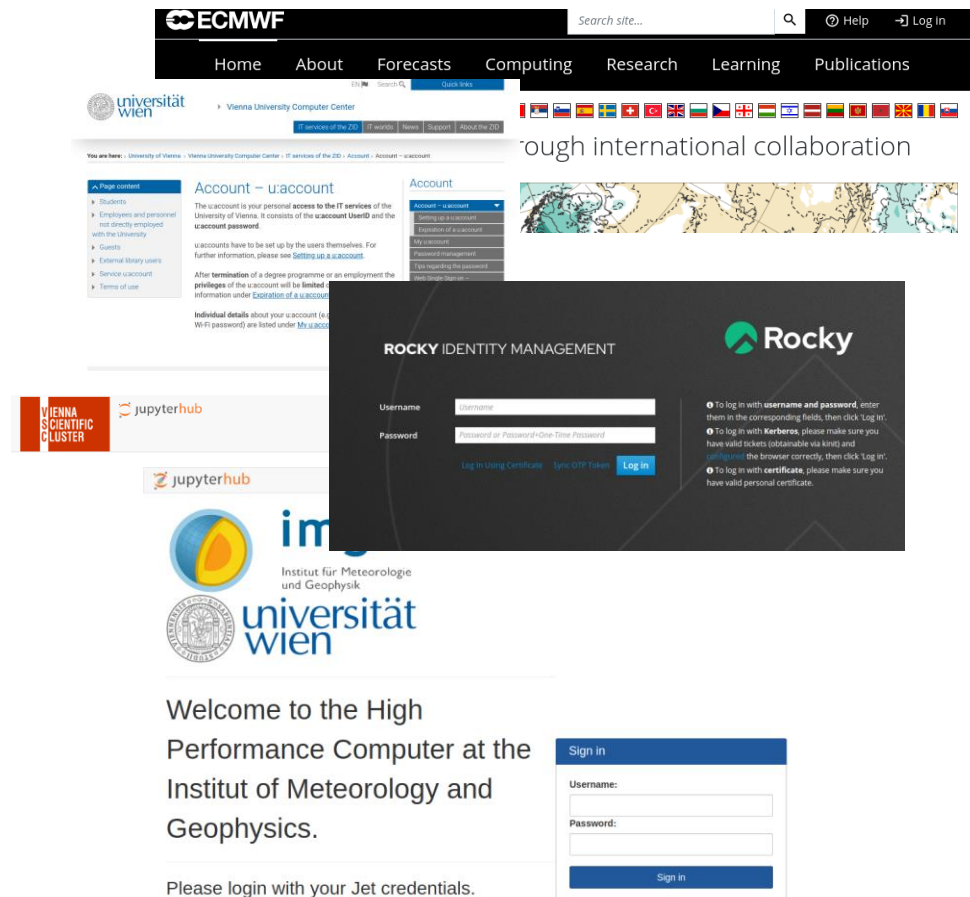
2. w:account (Wolke IMG account)

- All servers
- Jupyterhub on JET

3. ~~t:account~~ TeachingHub

4. ec:account (ECMWF)

5. vsc:account (VSC)

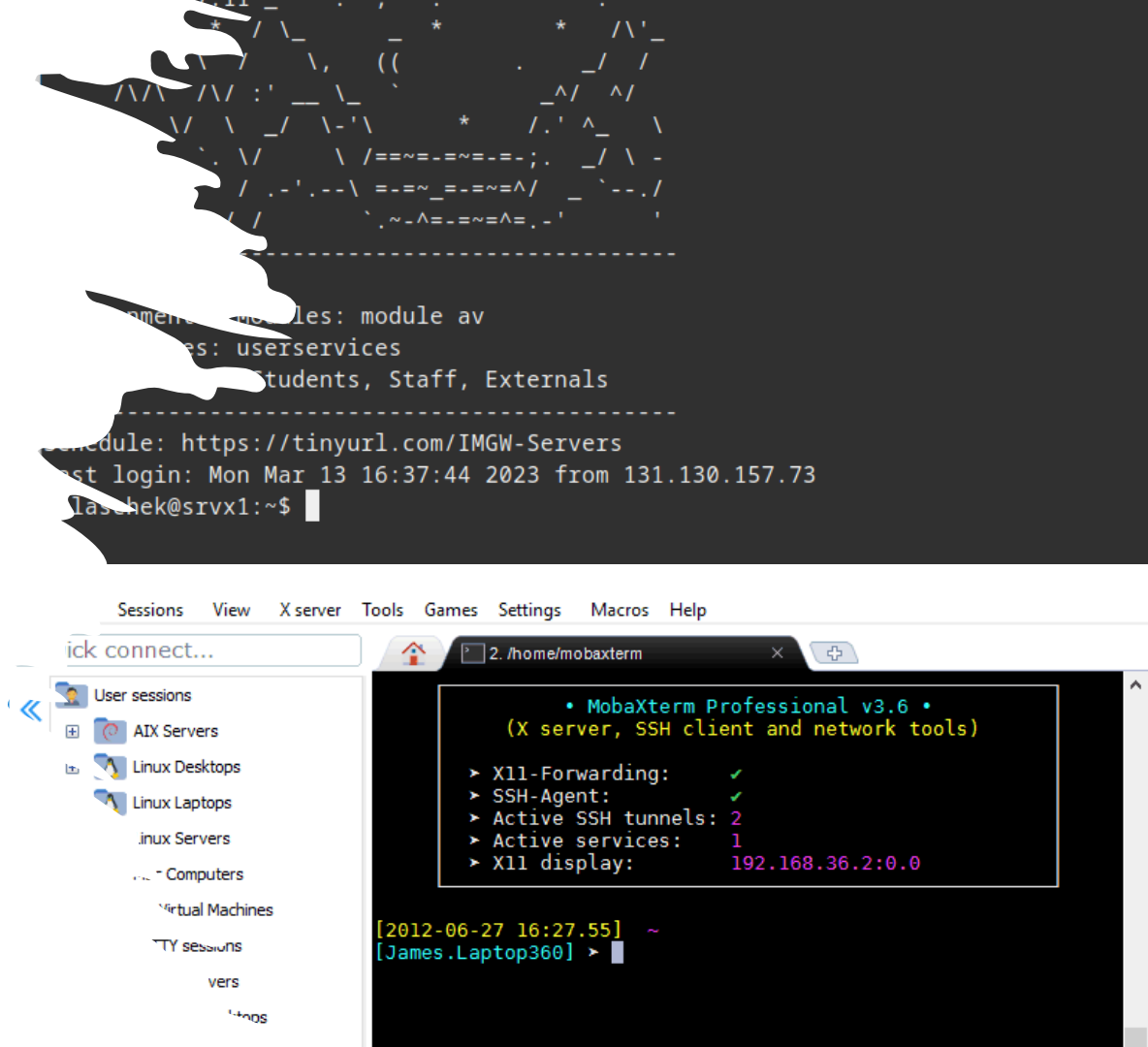


The collage displays four distinct login interfaces:

- ECMWF:** Features a navigation bar with links like Home, About, Forecasts, Computing, Research, Learning, and Publications. It includes a search bar and a 'Log in' button.
- Universität Wien:** Shows the 'Vienna University Computer Center' page with a sidebar for 'u:account' and a main content area explaining account usage and password management.
- Rocky Identity Management:** A dark-themed login page with fields for 'Username' and 'Password', and a 'Log in' button. It includes instructions for logging in with username/password, Kerberos, or certificates.
- Institut für Meteorologie und Geophysik:** A white-themed page with the text 'Welcome to the High Performance Computer at the Institut of Meteorology and Geophysics.' and a 'Sign in' button. Below the text, it says 'Please login with your Jet credentials.'

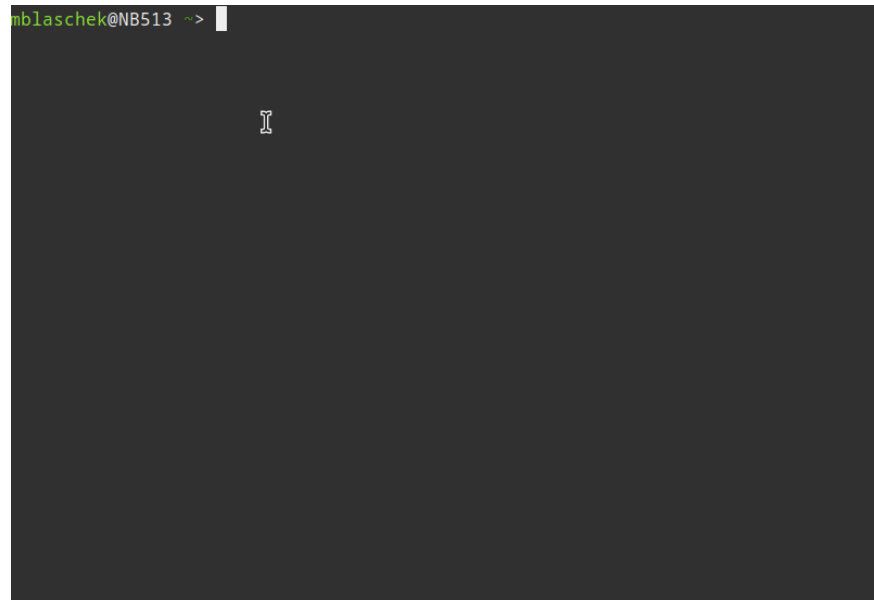
Shells & tools – Connection 101

- 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)



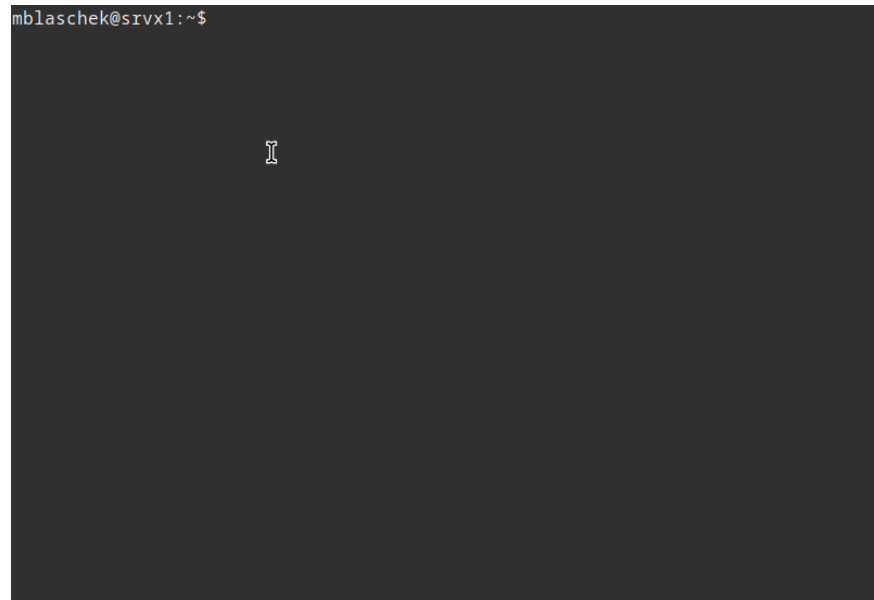
Shells & tools – userservices

- **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



Shells & tools – userservices filesender

- **userservices** – collection of useful scripts
 - **filesender** – [ACOnet](#) 250 GB
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Shells & tools – userservices ~~sshtools~~

- **userservices** – collection of useful scripts
 - **fi** – file manager + 250 GB
 - **qu** – quick transfer
 - **st** – *Has been replaced and is available now all the time* **stager**
 - **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
 - **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:~$
```



Shells & tools – userservices vnc (JET01, AURORA)

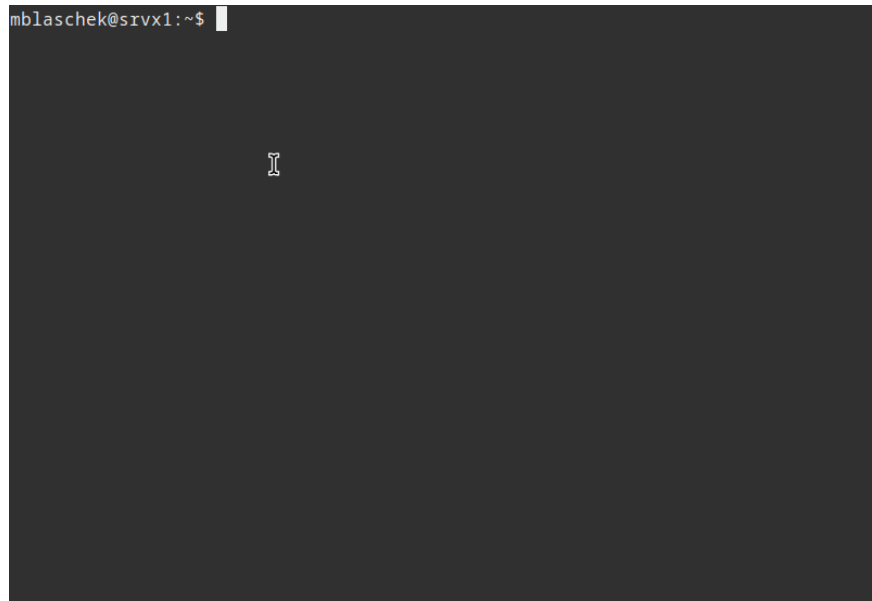
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 - **yopass** – encrypt messages
 - **vnc** – Virtual desktop on SRVX8
 - **weather** – current weather info

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

```
I
```

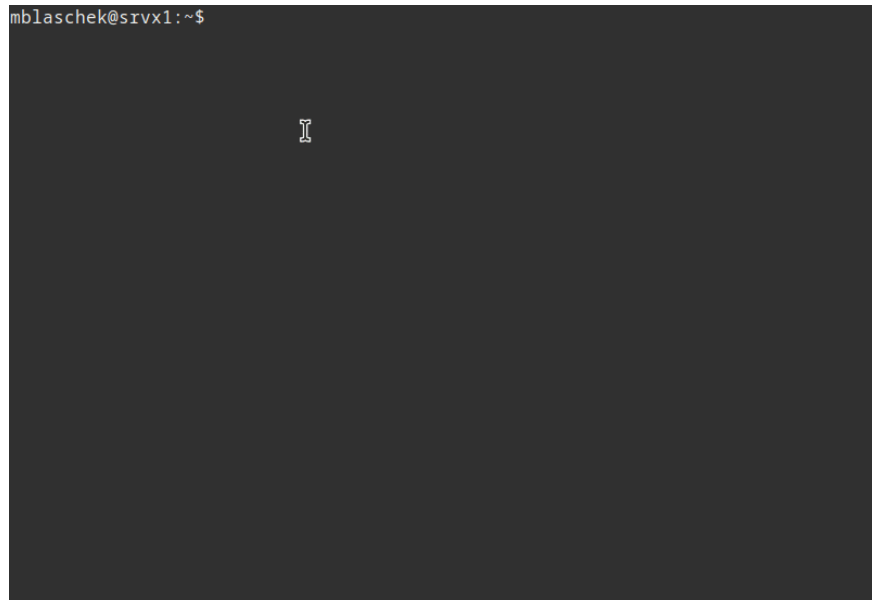
Shells & tools – user support

- 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`



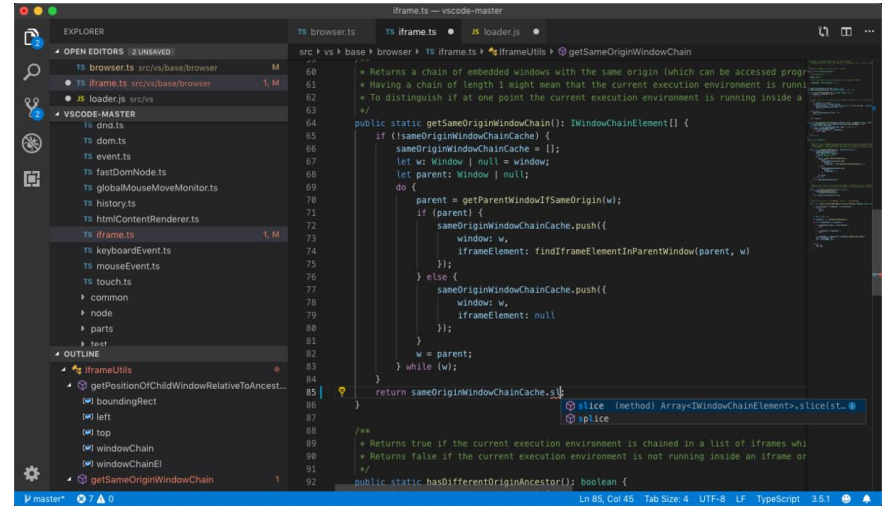
Shells & tools – user support

- 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

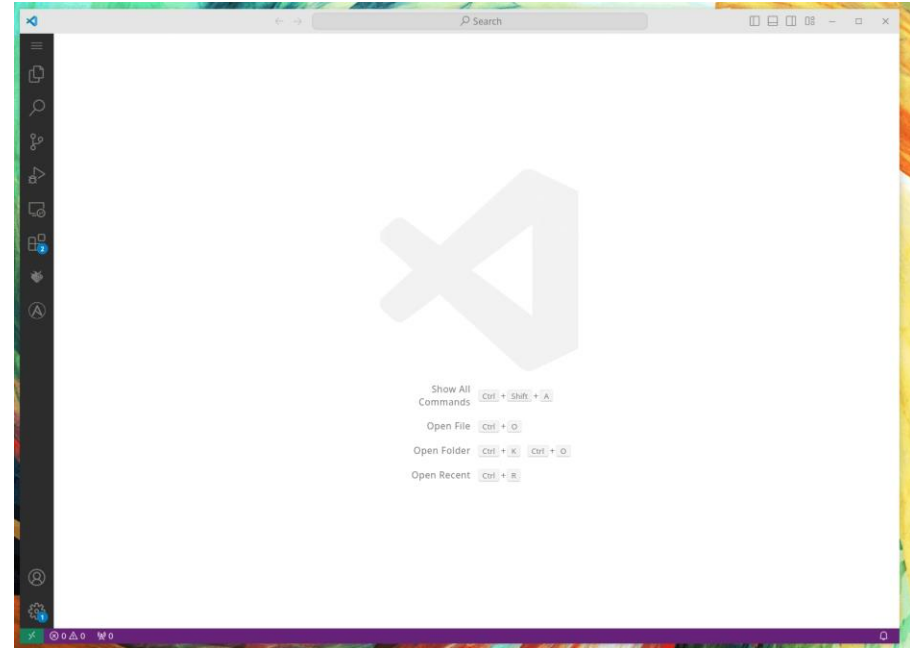
- Editors: **vim**, nano
- Dev Environment: **VSCode**, Code OSS
 - Extensions: Remote SSH, Dev Containers, Python, Notebooks, Modern Fortran, ...
 - Git fully integrated
- Python: build your own environment
 - Use conda or **micromamba**
 - Install packages, create environment file for a working environment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



```
src > vs > base > browser > TS iframe.ts > JS loader.js > @getSameOriginWindowChain  
//  
/*  
 * Returns a chain of embedded windows with the same origin (which can be accessed programmatically)  
 * Having a chain of length 1 might mean that the current execution environment is running inside an iframe  
 * To distinguish if at one point the current execution environment is running inside an iframe or not  
 */  
*/  
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(0, 1);  
}  
/**  
 * Returns true if the current execution environment is chained in a list of iframes which  
 * Returns false if the current execution environment is not running inside an iframe or  
 * otherwise  
 */  
public static hasDifferentOriginAncestor(): boolean {  
    return !getSameOriginWindowChain().length;  
}
```

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)



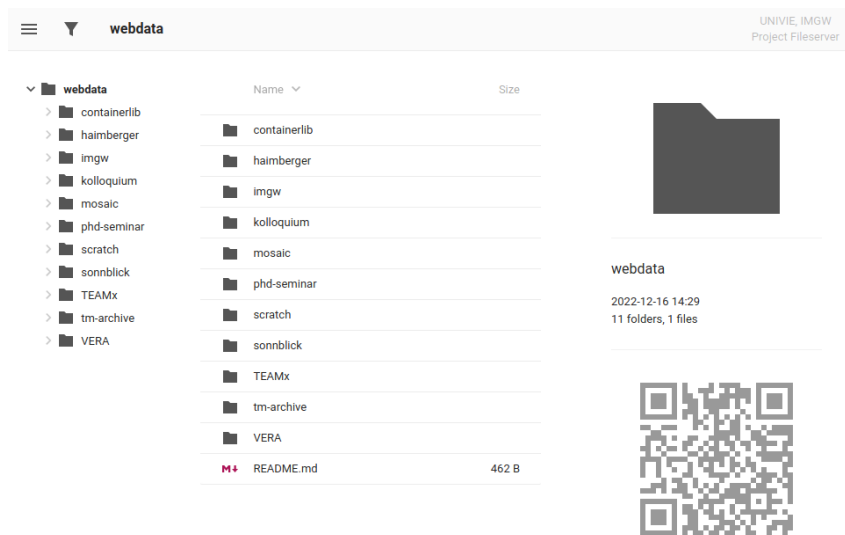


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clouds and services

@IMG, @ZID, ...

Clouds and services – webdata



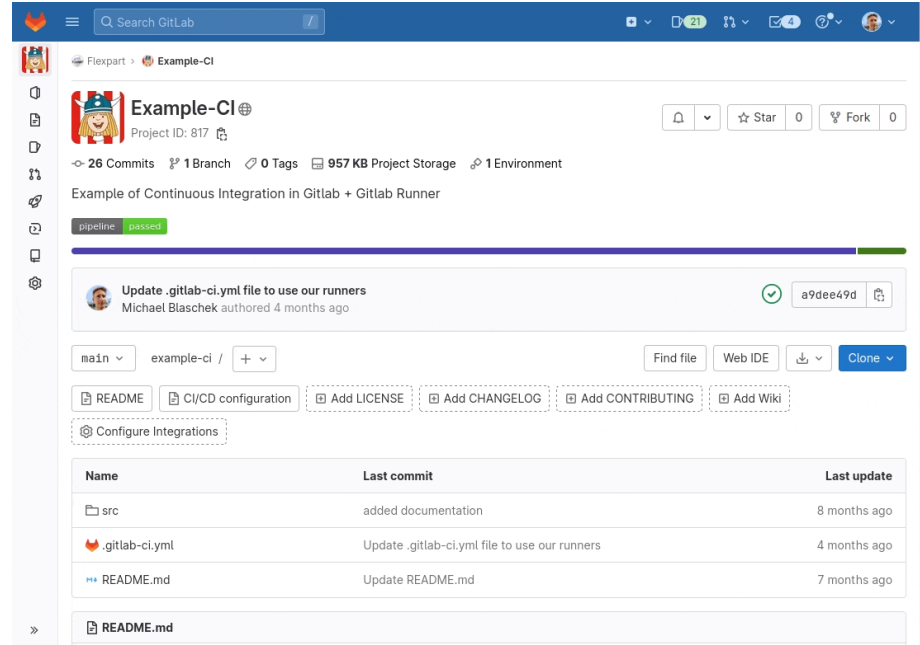
The screenshot shows a web-based file manager interface for a directory named 'webdata'. The top bar indicates the location is 'UNIVIE, IMGW Project Fileserver'. On the left, a sidebar shows a tree view of the directory structure. The main area displays a table of files and folders. A folder icon is shown above the table, and a QR code is displayed below it.

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

- 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>



The screenshot shows the GitLab web interface for a project named 'Example-CI'. The project is owned by 'Flexpart' and has a Project ID of 817. It shows 26 Commits, 1 Branch, 0 Tags, 957 KB Project Storage, and 1 Environment. The project description is 'Example of Continuous Integration in Gitlab + Gitlab Runner'. A pipeline is shown as 'passed'. A commit titled 'Update .gitlab-ci.yml file to use our runners' by Michael Blaschek is highlighted. Below the commit, there are buttons for 'Find file', 'Web IDE', and 'Clone'. 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 (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.

```
Tilix: [mosh] spack@srvx1~  
  
1 / 1 ▾ + ⏎ 📄  
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  
mbblaschek@srvx8:~/scratch$ cd test  
mbblaschek@srvx8:~/scratch/test$ ls  
Singularity.simple  
mbblaschek@srvx8:~/scratch/test$ ll  
total 4.0K  
-rw-r--r-- 1 mbblaschek vscusers 177 Oct 8 20:51 Singularity.simple  
mbblaschek@srvx8:~/scratch/test$ clear  
mbblaschek@srvx8:~/scratch/test$ ll  
total 4.0K  
-rw-r--r-- 1 mbblaschek vscusers 177 Oct 8 20:51 Singularity.simple  
mbblaschek@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 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)

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 ...

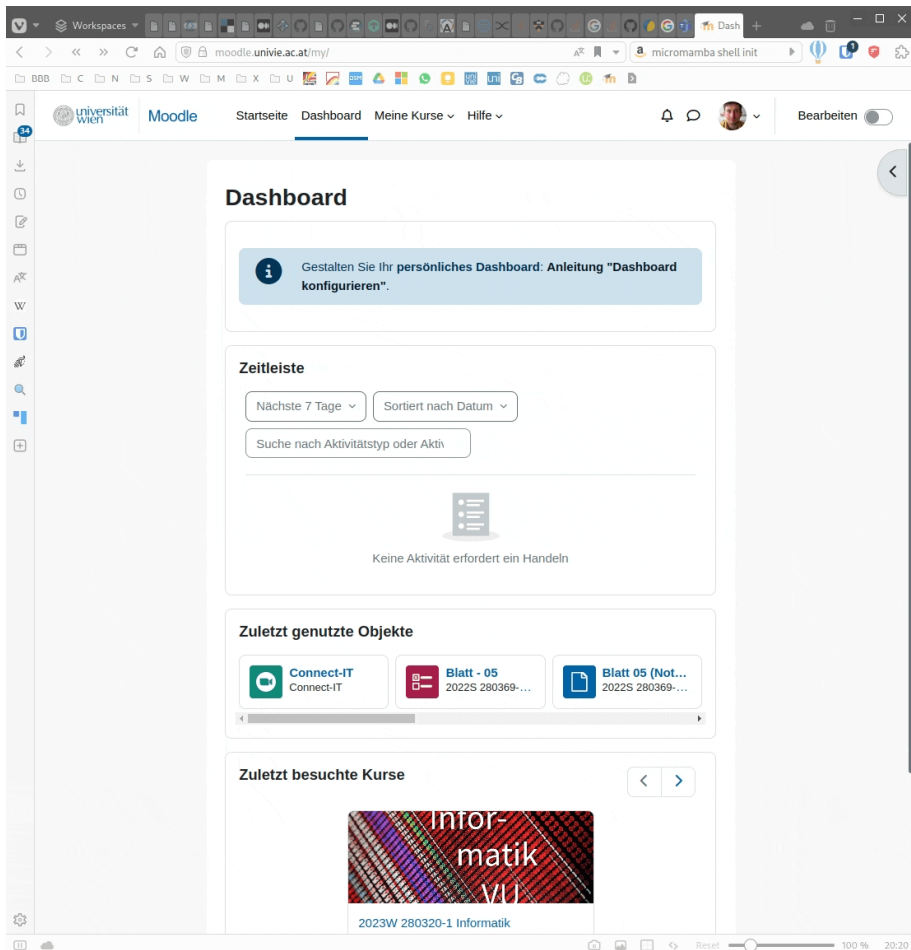
Vorkonfiguriertes Tool ⓘ + ⓘ ✕

Tool-URL ⓘ

✔ Tool-Konfiguration verwenden: Jupyterhub (Meteorologie)

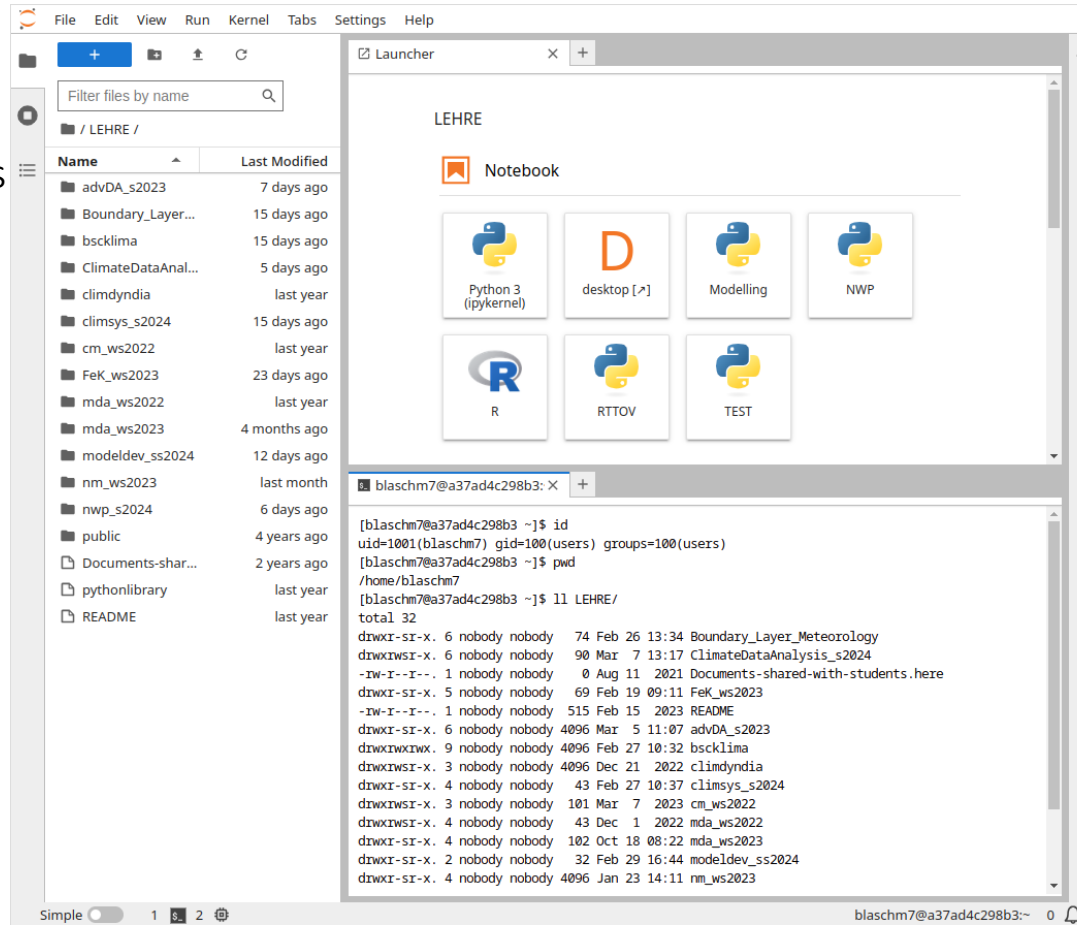
Resources – Jupyter

- Jupyter Notebook Server (Hub):
 - 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



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 $\neq$ teaching hub user
- Transfer files (**scp**, download) or userservices transfersh [file] + wget
- **Purge every September** (how to communicate to users?)



The screenshot displays the Moodle Jupyter Hub interface. On the left, a file browser shows the directory structure of the $\$HOME/LEHRE$ directory, which maps to $/srvfs/lehre$. The file list includes various directories and files, such as `advDA_s2023`, `Boundary_Layer...`, `bscklima`, `ClimateDataAnal...`, `climdyndia`, `climsys_s2024`, `cm_ws2022`, `FeK_ws2023`, `mda_ws2022`, `mda_ws2023`, `modeldev_ss2024`, `nm_ws2023`, `nwp_s2024`, `public`, `Documents-shar...`, `pythonlibrary`, and `README`. The right panel shows the 'Launcher' window, which displays a grid of icons for different environments: Python 3 (ipykernel), desktop [^], Modelling, NWP, R, RTTOV, and TEST. Below the launcher, a terminal window shows the output of the `id` command, indicating the user is `blaschm7` with a `uid=1001(blaschm7)` and `gid=100(users)`. The terminal also shows the `pwd` command output, which is `/home/blaschm7`. The terminal output for the `ls -l` command shows the contents of the `LEHRE` directory, including files like `Boundary_Layer_Meteorology`, `ClimateDataAnalysis_s2024`, `Documents-shared-with-students.here`, `FeK_ws2023`, `README`, `advDA_s2023`, `bscklima`, `climdyndia`, `climsys_s2024`, `cm_ws2022`, `mda_ws2022`, `mda_ws2023`, `modeldev_ss2024`, and `nm_ws2023`.

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



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



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
 - 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!!!!**





Communication is keen

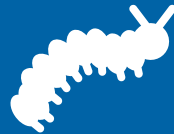
1. Check documentation (*talk to yourself*)  
2. Ask a colleague (*talk to another person*)  
3. Ask IT (*talk to a group*)  

Contact IT

VSC related? >> Me

Server related? >> Me

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





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Questions?

PhD seminar

Bare metal, shells and clouds – MB

On the wiki:
tutorials – Computing

