

...









The speakers

Ronald Maier

Ronald Maier has been <u>Vice-Rector for Digitalisation and Knowledge Transfer</u> at the University of Vienna since 1 October 2019. He is Professor of Information Systems at the University of Innsbruck.

Ulf Busch

Ulf Busch has been CIO of the University of Vienna since 2010. He is the Head of Zentraler Informatikdienst.

Leopold Haimberger

Leopold Haimberger is Professor of Meteorology and Vice Dean for Infrastructure at the Faculty for Geosciences, Geography and Astronomy.





The speakers

Simon Engelberger

Simon Engelberger studied zoology at the University of Vienna. Since 2020 he is the Collections Manager in charge of the University of Vienna Zoological Collection.

János Békési

János Békési is at the ZID since 2017, supervising UNIDAM, a digital asset management system realized with Easydb, and several services for researchers mainly in the digital humanites.

Thomas Rattei

Thomas Rattei is Head of the Division of Computational Systems Biology and Vice-Head of the Department of Microbiology and Ecosystem Science.





The speakers

Ulrich Kiermayr

Ulrich Kiermayr is Head of Communication Networks & Infrastructure and Vice Head of Zentraler Informatikdienst.

Eva Karall



Eva Karall is Head of E-Learning at <u>Zentraler Informatikdienst</u>. The staff unit is responsible for the technical support and further development of the e-learning platform <u>Moodle</u> and tools for digital teaching (BigBlueButton, <u>Zoom</u>) as well as the <u>u:stream</u> services at the University of Vienna.



Michaela Bociurko, Moderator

Michaela Bociurko is Head of IT Communications and Marketing at Zentraler Informatikdienst.

Sara Curtis, Moderator Sara Curtis is a member of the IT Communications and Marketing team at <u>Zentraler Informatikdienst</u>.







The topics

Opening

• Ronald Maier

• Ulf Busch

Innovative IT solutions in selected scientific projects



- IT for Meteorology and Climate Science, Leopold Haimberger
- Digitalisation of zoological specimens, [...] held by the zoological collection of the University of Vienna, Simon Engelberger, János Békési
- DataLife Data Infrastructure for Life Sciences, Thomas Rattei

IT services of the ZID for science and research

- Supporting projects in all stages, Ulrich Kiermayr
- Overleaf Collaborative Online LaTeX Editor, Eva Karall

Summary and Outlook

• Ronald Maier











Opening

- Ronald Maier
- Ulf Busch







Innovative IT solutions in selected scientific projects

- IT for Meteorology and Climate Science
- Digitalisation of zoological specimens, historical photographs and other archival materials held by the zoological collection of the University of Vienna (UVZC)
- DataLife Data Infrastructure for Life Sciences







IT for Meteorology and Climate Science

Presentation by Leopold Haimberger





Outline

• Our research topics

- Data assimilation
 - How to get satellite and weather observations onto a model grid
- Climate Data Analysis and Climate Modeling
- Ensemble forecasts
- Monitoring trace substances
- Our computing environment
- Contributing to FAIR data
- Towards cloud computing
- Challenges



Analysis = corrected description of the atmosphere in model space





Our local resources

Bare metal @ Department – SRVX – JET – VSC Nodes



Main External computing facilities

ECMWF+Copernicus

- reliable partner since decades
- HPC and 100 PB data archive

K-computer (Japan) 1000 member forecast ensemble

- HPC software stacks (FORTRAN, MPI, OpenMP, Python)
- Jupyter hubs on local servers and VSC
- Both for research and teaching





PHAIDRA, GitLab and Mattermost, Confluence – Don't switch it off!

- Phaidra for long-term archiving of climate model data and analysis scripts
- GitLab for code development and project management (incl. external collaborators)
- Mattermost for fast internal communication
- Departmental Wiki pages for internal administration and communication



PHAIDRA













Copernicus Climate Reanalysis – ERA5

- Gridded 3D atmospheric data set of the past 80 years (1940-)
- Ideal to learn about the state and evolution of recent climate
- Quality-certified, free download via Copernicus
- ~10 PB, 3000 cites/year, hugely popular
- We have copied small fraction, would like to have more, already uses 15% of our disk space.





Wikimedia commons





Publishing@Copernicus

- Data store has all ingredients of a FAIR data repository
- Very liberal license
- Copernicus takes care of data lifecycle
- But where is the logo?
- Should we have published it on PHAIDRA?



- **Bundle Geoscience IT resources in Austria Cloud4GEO**
- **Create** a powerful distributed cloud for geospatial data processing
- Single Sign-on
- Focus on interoperability: Open Standards
- Link to EOSC and EGI, Copernicus
 - not only as user, but also
 - share our data there (also compute)
- FAIR gives credit, attracts users!
- Data are "near": high bandwidths, low latency
- Expensive to build and maintain















Are there other choices?

- Run our codes where the data are.
- Copernicus DIAS (e.g. **WEkEO** https://www.wekeo.eu/about)
- Free Trial
- Access via JupyterHub, VM
- Provides harmonised, high bandwidth data access to many PB of EO data
- Data free, only computing costs
- Some teething troubles, but improving.
- Next Generation:



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GPUs				-	1	2
Trial period	5 Institutiona	I Private sector users	Research & civil society	1 month	-	-





Business likes FAIR data!

- Copernicus' aim is to support companies with climate and monitoring data
- Well received by small companies in Europe ...
- but also the big fishes ...
- Google and Amazon hold copies of ERA5

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Google Cloud Overview Solutions Products Pricing Resources
Cloud Storage Overview Guides Reference Samples Support Resources
≂ Filter
Cloud Storage Documentation > Resources All resources ERA5 data





- Well supported cloud environment
- 23 USD/TB/month
- 70,000 USD for 300 TB per year

We will not buy from them!

Google Cloud

Pricing tables

Timportant: Pricing updates for Cloud Storage took effect on Oct. 1, 2022 and on Apr. 1, 2023.

The pricing tables below show what charges apply when using Cloud Storage.

North America South America	Europe Midd	le East Asia	Indonesia Australia	
Location	Standard storage (per GB per Month)	Nearline storage (per GB per Month)	Coldline storage (per GB per Month)	Archive storage (per GB per Month)
Warsaw (europe-central2)	\$0.023	\$0.013	\$0.006	\$0.0025









What Google does with ERA5

Train AI (GNN) for weather forecasting







"We also thank ECMWF for providing invaluable datasets for the research community"

GraphCast: Learning skillful medium-range global weather forecasting

Remi Lam^{*,1}, Alvaro Sanchez-Gonzalez^{*,1}, Matthew Willson^{*,1}, Peter Wirnsberger^{*,1}, Meire Fortunato^{*,1}, Alexander Pritzel^{*,1}, Suman Ravuri¹, Timo Ewalds¹, Ferran Alet¹, Zach Eaton-Rosen¹, Weihua Hu¹, Alexander Merose², Stephan Hoyer², George Holland¹, Jacklynn Stott¹, Oriol Vinyals¹, Shakir Mohamed¹ and Peter Battaglia¹ ^{*}equal contribution, ¹DeepMind, ²Google







Conclusions

- We like the UNIVIE RDM tools a lot!
- Power of FAIR EO data quickly unfolding
 - Data assimilation plays an important role
 - We are small players, but let the big picture shine a little more
- Frequent quick scans through large amounts of data
- We need affordable "near" cloud computing service
 Build one for EO in Austria ongoing
 - Tap into European resources just starting
- Strong winds of change AI challenge
 - Do we invest wisely, can we adapt quickly enough?





© Image by Suez Canal Authority / AP

© Image by https://www.flickr.com/ photos/jnandreae/)





Questions about IT for Meteorology and Climate Science?

• Please ask your questions as a chat comment.











Digitalisation of zoological specimens, historical photographs and other archival materials held by the zoological collection of the University of Vienna (UVZC)

Presentation by Simon Engelberger and János Békési





AV Media







AV Media: Standards

- Standard: Audiovisual Core (Audubon Core), AC
- Controlled Vocabularies
 - AC
 - Art & Architecture Thesaurus® (AAT)

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AV Media: Interlinks

• Linked with digitised Card Files



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AV Media: Linked bibliographic data

• Linked with YARM Reference Manager

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AV Media: Person IDs

- Controlled list of persons
- Including wikidataID for all persons



X : Adensamer, Wolfgang 1899 - 1964 Person #51682 **Biographische Daten** Geburtsjahr Geburtstag Geburtsmonat 5 1899 Sterbetag Sterbemonat Sterbejahr 4 1964 Daten vollständig Literatur OID_L_web • https://www.wikidata.org/wiki/Q107163002 🗗 Thesis UW-Archiv, PH RA 5817: Aus Zoologie: "Über den Bau der

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Mundteile von Scutigerella immaculata Newp.", 1924.01.09-1924.01.16 (https://scopeq.cc.univie.ac.at/Query /detail.aspx?id=259980)

Future steps

- DWCA export (xml/csv)
- AC export (xml/csv)
- Link with GBIF Taxonomic Backbone (Global Biodiversity Facility, <u>https://www.gbif.org/</u>)
- Automated export of DWCA dataset to GBIF

© Image by <u>https://www.gbif.org/</u>







ZID-related: Infrastructure

- Virtual machine in ZID virtual infrastructure (with backup and monitoring)
 - Presently 4 CPUs, 12 GB RAM and 1 TB storage
- Several Docker containers comprise easydb functionality
- File system storage
- Update by pulling new docker images (every 2–3 weeks)
- Mirrored development instance for tests and try-outs (plugins)







ZID-related: Components/containers

- File server ("Eas") in C
- Elasticsearch
- Postgresql
- Base server in Python
- Web frontend in Coffeescript/Javascript











ZID-related: Access and data

Access by other means than by browsers

- Plugins for web frontend (Coffeescript)
- Plugins for server and/or API (Python)



© Image by storyset on Freepik

Current data

- 16,000 images
- 54 object types (mainly imported helper objects, 7 main objects)
- 56,000 objects (e.g. taxon or YARM entries) in total





ZID-related: easydb

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Data model

 Specimen object type has about 90 fields





ZID-related: Data refining

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• Data is **refined/processed** in Jupyter notebooks and exported as CSV files

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ZID-related: Import of metadata

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• Metadata are imported and/or bulk updated as **CSV files**

URLs and workflow

- URLs of interest:
 - Documentation of easydb: <u>https://docs.easydb.de/en/</u>
 - General info for easydb: <u>https://www.programmfabrik.de/en/easydb/</u>
- Our workflow: Nothing special → e-mail, telephone, feedback loops, try-outs
- Contact:
 - <u>simon.engelberger@univie.ac.at</u>
 - janos.bekesi@univie.ac.at







© Image by storyset on Freepik

Questions about Digitalisation of archival materials?

• Please ask your questions as a chat comment.















Presentation by Thomas Rattei

DataLife – Data Infrastructure for Life Sciences





Data in Life Sciences

- Huge data collection in short time:
 - Biological and medical imaging
 - Real-time microscopy
 - DNA and RNA Sequencing
 - Chemical analytics
- Interpretation with machine learning and artificial intelligence
 - Transformation of data into features
 - Real-time access to large data for training
 - Compute-intensive learning



 $\ensuremath{\mathbb{C}}$ Image by full vector on Freepik





Example: Genome data







Future needs: data-intensive projects

• FWF Cluster of Excellence "**Microbiomes Drive Planetary Health**" Centre for Microbiology and Environmental Systems Science et al.

ERC Advanced Grants

- -Manuel Zimmer
- -Michael Wagner

• Wittgenstein Awards

- -Christa Schleper
- -Michael Wagner







Data acquisition, storage and processing



PromethION 48 Specification:

Sequencer:

• H 190 x W 590 x D 430 mm, 25 kg

Data Acquisition Unit:

• H 440 x W 178 x D 470mm, 25 kg

Compute spec:

- 64 TB SSD Storage
- 384 GB RAM
- Intel CPU
- 4 x GV100 basecall accelerators

© Image by Goenka et al., Nature 2022





Now: Life Science Compute Cluster







Next: DataLife project



Funding by BMBWF in "Digital Infrastructures" initiative. Total costs 2.5 mio, ministry contribution 1.8 mio.





Data creation sites

- Ahrends group Metabolomics/Lipidomics (Chemie 1090)
- BioOptics Facility (Max Perutz Labs DBG VBC5)
- EDGE (UZA2 1090)
- EM Facility (IST Austria)
- EM Facility (VBCF)
- FACS Facility (Max Perutz Labs)
- Gerner group Proteomics (Chemie 1090)
- Joint Microbiome Facility / BSF (Anna Spiegel Building CeMM)
- Joint Microbiome Facility / MedUni (AKH 5P)

- Joint Microbiome Facility / CMESS (UBB)
- MassSpec Facility (Max Perutz Labs / VBCF)
- Menche group (Max Perutz Labs (DBG VBC5))
- NGS Facility (VBCF / BSF Anna Spiegel Building CeMM)
- Pharmazie (UZA2 1090)
- Strukturbiologie (Max Perutz Labs (DBG VBC5)
- Zanghellini group Metabolic Modelling (Chemie 1090)
- Zimmer group (UBB)





Data processing sites

- Vienna Scientific Cluster
- CLIP/CBE of ÖAW
- CIBIV-Cluster at Max Perutz Labs
- Life Science Compute Cluster of University of Vienna (LeWi, CMESS, Chemistry and JMF)
- MedUni Wien Computing facilities
- Laboratory of Computational Biophysics highperformance cluster (Max Perutz Labs)
- Dorothy-Cluster (Max Perutz Labs, Structural Biology)







High-performance data storage

- GPFS Storage with IBM Active File Management (AFM), partially redundant
- Storage nodes with Flash-Disk ratio of 1:10







Network infrastructure

Data creation sites <-> Storage

- Fast(er) LAN connections
- Storage <-> Data processing sites
- Direct dedicated networks with multiple 100 Gbit/s Ethernet RDMA links

Side effects:

- Newly created redundant 100 Gbit/s between UBB and Arsenal via NIG and University Main Building
- Redundant 100 Gbit/s between Medical University resp. MeduniBackup and Arsenal (via NIG, via Campus3A/University Main Building)





DataLife work/time plan

- 1. Concept (2023)
- 2. Planning (2023/24)
- 3. Realization (2023/24)
- 4. Operation (2025/26)

Two additional FTE:

- Technician (ZID)
- Data Scientist (Vienna Biocenter)







Data management and harmonisation

Training of user community needed:

- Open Science
- FAIR principles
- Data lifecycles and storage economy
- Data standards

Help by:

- 2 data stewards
- LiSC Servicedesk



Outlook and further impacts

- Contribution to national and international infrastructure:
 - -European Open Science Cloud
 - -EURO-Bioimaging
 - -ELIXIR
- Formation of ELIXIR Austria node
- Contact: <u>thomas.rattei@univie.ac.at</u>













Questions about DataLife – Data Infrastructure for Life Sciences?

• Please ask your questions as a chat comment.











IT services of the ZID for science and research

- Supporting projects in all stages from development to execution
- Overleaf Collaborative Online LaTeX Editor







Supporting projects in all stages – from development to execution

Presentation by Ulrich Kiermayr

What we can offer

- Support in the project planning phase regarding the needed infrastructure
- Evaluation of options to meet project requirements
- Contact point for external support
- Contracts to use in procurement phase
- Technical support in the realisation of projects
- Monitoring and debugging in case of problems







Why this is important

- Vienna University's campus network is a complex system
- Constraints we need to meet
- Different options to achieve the goals of the project
- Additional services can be offered by the ZID
- Changes to the infrastructure require time (delivery times, cabling, setup times)
- Changes cost (a lot of) money, has to be taken into account in project proposals
- The infrastructure has to be managable on a large scale











What our infrastructure offers today

- 1 Gbit to every system
- 10 Gbit between locations
- 100 Gbit uplink to the internet (including other ACOnet participants like VSC)
- Redundancy in the core network (including several large university locations)







What is currently in the making

- Connecting large locations (UBB, UZA ...) via 100 Gbit to the core network
- Continuous upgrade to access infrastructure to allow more bandwidth inhouse
- Options for dedicated links between services like VSC







What can be done

- Increase of bandwidth
- Links to other locations
- 10 Gbit to dedicated systems
- Serverhousing for dedicated systems

Bear in mind: this needs money, people and time – so early planning and budget availability is key to a successful project.



Contact

- Via Servicedesk: **<u>Request about the data network</u>**
- Via service e-mail address: digital.zid@univie.ac.at
- Directly: <u>ulrich.kiermayr@univie.ac.at</u>, <u>christian.kracher@univie.ac.at</u>



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Questions about Supporting projects in all stages?

• Please ask your questions as a chat comment.















Overleaf – Collaborative Online LaTeX Editor

Presentation by Eva Karall





Why LaTeX and how does it work?

- Developed by Leslie Lamport in the 1980s, LaTeX came to its name: ${
 m La}$ mport ${
 m TeX}$
- A markup language that facilitates the production of well-formatted documents







What is Overleaf?

- Overleaf is an online LaTeX editing tool that
 - allows you to create LaTeX documents directly in your web browser
 - "compiles" your LaTeX automatically to show you the results

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Which license do I get?

- **Students** of the University of Vienna receive an **Overleaf Free license**:
 - –Unlimited number of projects
 - -Collaborating in real time with another person
 - -Using templates



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 - unlimited number of authors for documents
 - full version history
 - synchronization with e.g. Git/GitHub

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Templates

- Gallery with thousands of templates
- Anyone can submit projects for possible inclusion in the gallery
- Templates available for thesis, CV or submission to scientific journals and conference, e.g. the IEEE¹ and Springer
- Official **University of Vienna templates** available

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Sharing

- Every document you create on Overleaf is private by default
- Two ways to share your work with collaborators:
 - By private invitation
 - Private invitations allow you to invite selected, named collaborators to access your projects
 - the number of named collaborators you can invite on each project depends on your plan
 - By link-sharing
 - Link-sharing allows you to share your projects via secret links for viewing, commenting and editing



Screenshot: www.overleaf.com/learn/how-to/Sharing_a_project





Collaboration

- Single master version of each document
- Simultaneous collaborative editing
- Discussing within Overleaf
- Tracking all changes
- Keeping one to-do list
- Accepting and rejecting changes

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Screenshot: https://www.overleaf.com/blog/track-changes-and-comments-in-latex-2017-03-09

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More information

- Service page <u>zid.univie.ac.at/en/overleaf/</u>
- University of Vienna on Overleaf <u>www.overleaf.com/edu/univie</u>
- Instructions and support via Overleaf
 - <u>Documentation</u> of Overleaf
 - Helpful <u>how-to guides</u>
 - Technical support via <u>contact form</u> or e-mail to <u>support@overleaf.com</u>











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Thank you for your attention!

