MIAPPE Wizard: Enabling easy creation of MIAPPE-compliant ISA metadata for Plant Phenotyping Experiments

Sebastian Beier (FZ Jülich) and Daniel Arend (IPK Gatersleben)

miappe Wizard

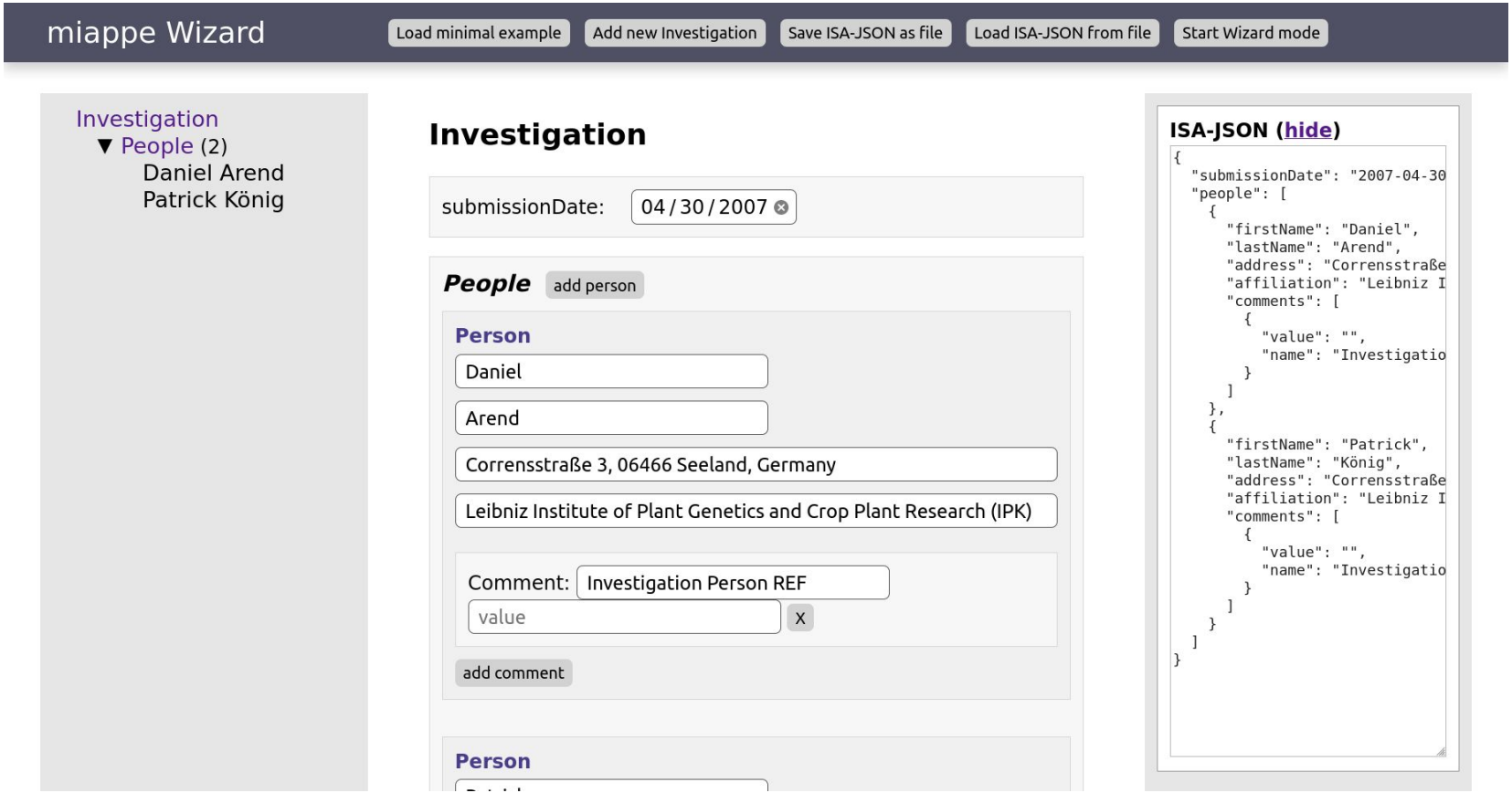
Motivation: Build web app to generate metadata for plant phenotypic experiments

- Tight collaboration with Data PLANT @nfdi4plants

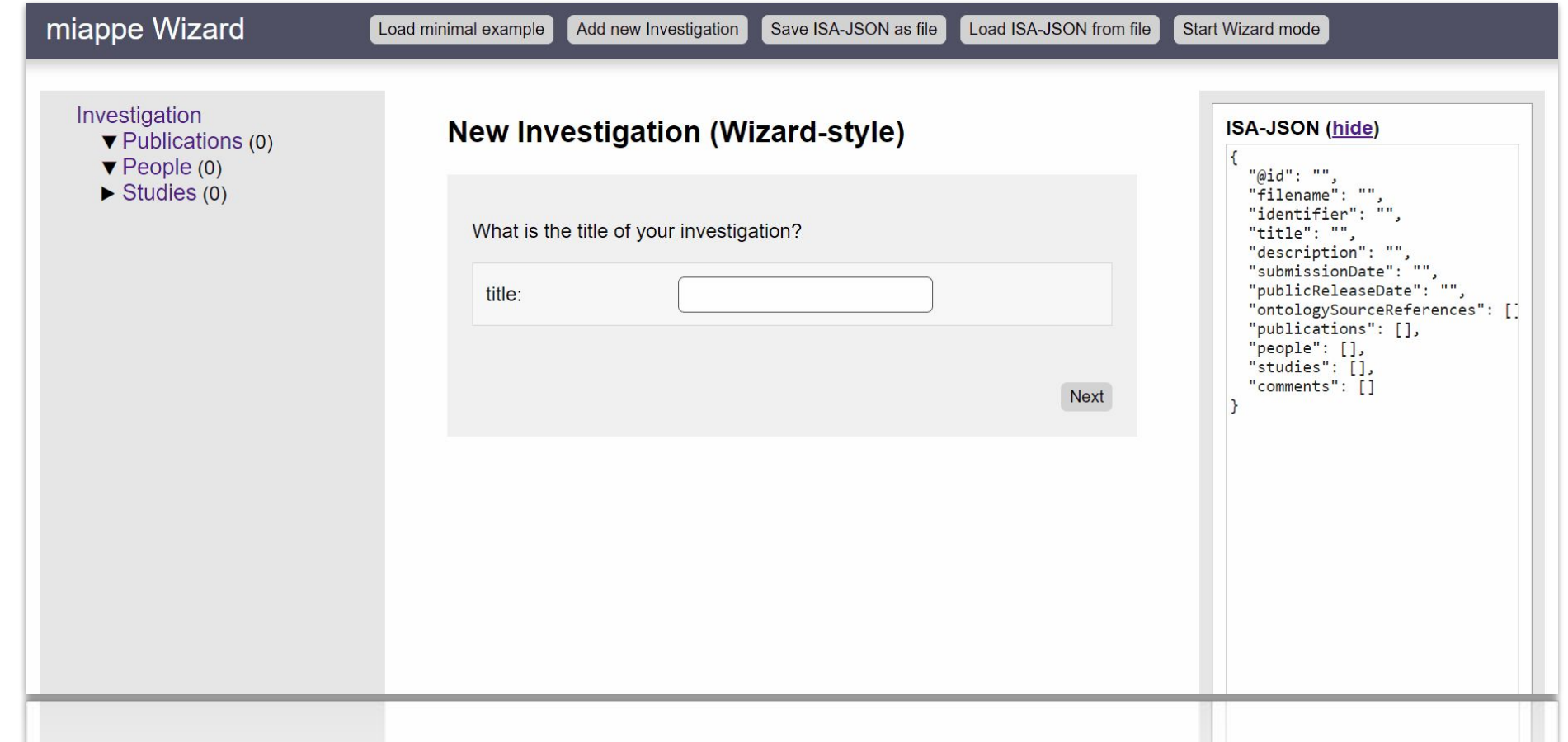
- Tasks:
  - Graphical design
  - User experience
  - Data model discussions (ISA / MIAPPE)
  - Ontology connections (DataPLANT, MIAPPE, CRediT, others)

  - … and of course having fun!

Prototype GUI

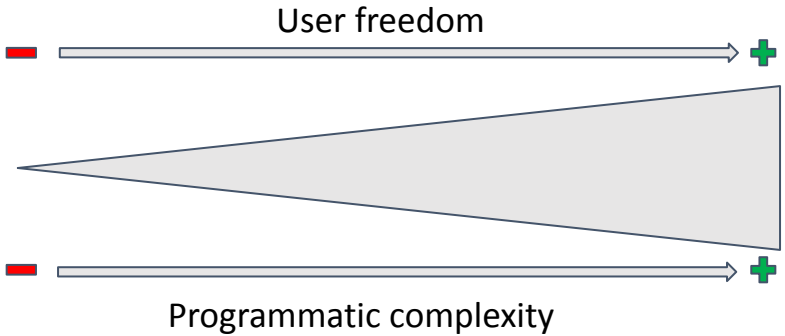


Wizard questionnaire



Challenges

- ISA-Tab - ISA-JSON differences (hierarchy, identifier names)
  - MIAPPE (phenotyping standard) mapped to ISA-Tab but not to ISA-JSON
- Difficult to accommodate all user groups (balance between novice and experts)



- Incorporating virtual participants → limiting to certain time slots
  - Discussion Wednesday afternoon (ISA & MIAPPE)
- Connecting into other tool ecosystems (ARC Commander, pISA-Tree)

Current progress

Motivation: Build web app to generate metadata for plant phenotypic experiments

- Status:
  - Graphical design
    - Basic design (optional developer console)
    - Treeview
  - User experience
    - Form based and questionnaire dialog
  - Data model discussions (ISA / MIAPPE)
    - Generic ISA → future perspective MIAPPE
    - ISA implementation (ISA-JSON) to be discussed with community
  - Ontology connections (DataPLANT, MIAPPE, CRediT, others)
    - REST API adaptors to DataPLANT ontology
    - Extension of DataPLANT ontology to include MIAPPE & CRediT

Extending the NFDI4Microbiota Knowledge Base

Justine Vandendrope (ZB MED) and Kassian Kobert (Bielefeld University)

Bla Bla

de.NBI
GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE

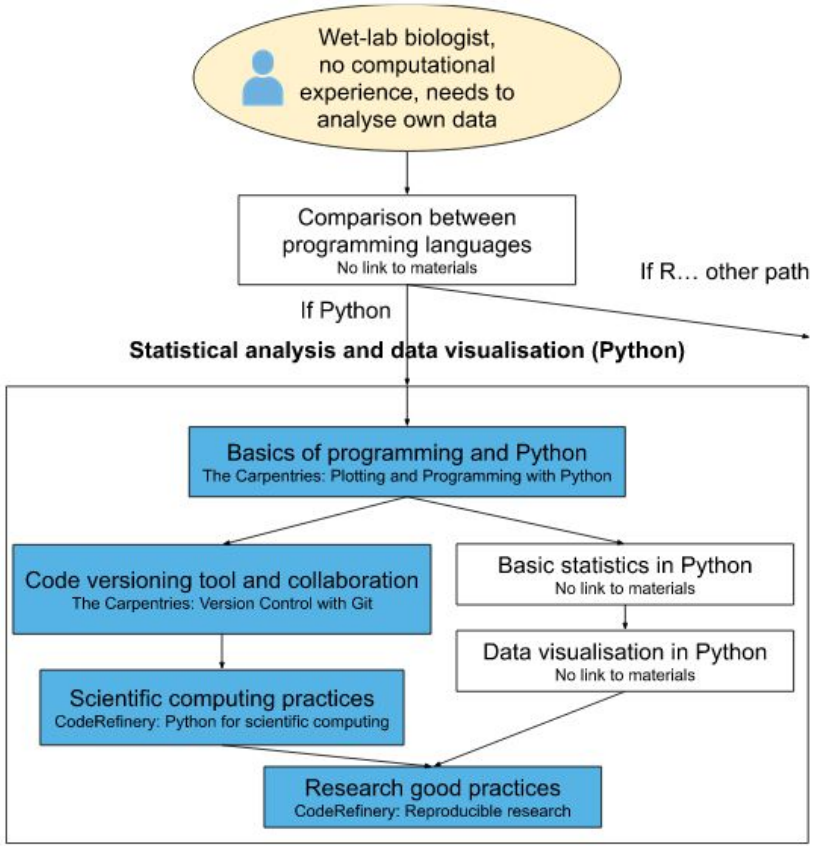
elixir
GERMANY

Mapping the training journey in Bioinformatics and beyond

Lisanna Paladin (EMBL Heidelberg) and Pablo Mier (University of Mainz)

Quick recap

- **Aim**: mapping the **“training journey”** of different **personas** in Bioinformatics, visualising the steps needed to acquire expert knowledge in each topic, or skill.
- **For**: trainers & trainees.
- **How**: training paths



1. Gathering data: Strategy

- About
  - Personas: ”Wet lab biologist that is able to visualise small dataset“
  - Skills: ”Programming in R”, “Data visualisation (in R)”, “Programming in Python”
  - Training courses:

Introduction to R

Data Carpentry contributors

Python Essentials 1

Dive into programming, learn Python from scratch, and prepare for the PCEP – Certified Entry-Level Python Programmer certification.

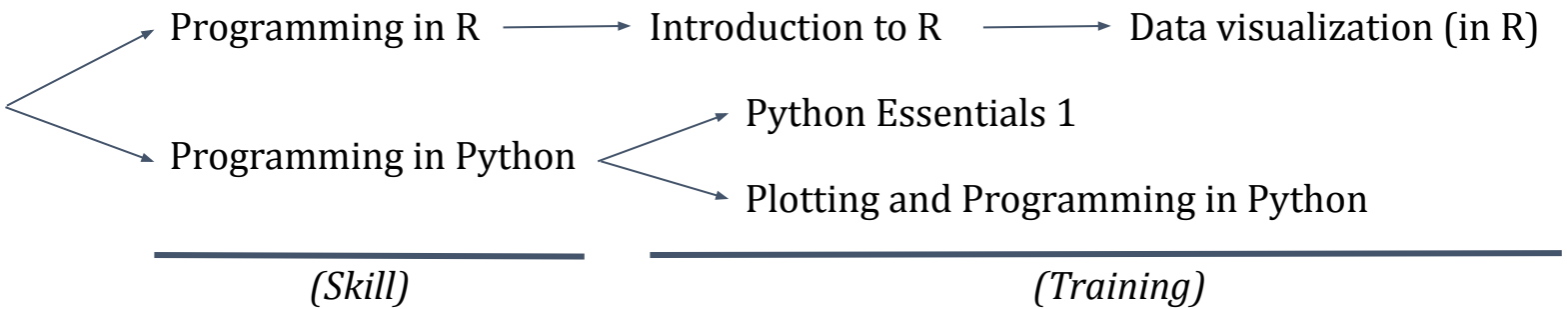
Data Visualization

This lesson shows how to choose the appropriate graphic to represent your data and research question, inspired by Choosing a good chart, and then how to implement construction of the graphic using `ggplot2`.

Plotting and Programming in Python

This lesson is an introduction to programming in Python 3 for people with little or no previous programming experience. It uses plotting as its motivating example and is designed to be used in both Data Carpentry and Software Carpentry workshops. This lesson references JupyterLab but can be taught using alternative Python 3 interpreters as well (e.g., repl.it, Anaconda).

- Dependencies



1. Gathering data: Current status

18 personas (8 fields each)

Code	Persona SHORT description	Carreer stage	Skills they have already / background	Any programming skills?	Any background in life sciences?	Experience they already have	Need / motivation	Skills
P1	Wet lab biologist that is able to visualise small dataset	Early	Wet lab methods, life science background	No	Yes	Wet lab techniques	Visualise small dataset	S1|S36,S2,S3
P2	Biochemist who gets their transcriptomic dataset	Early	Biochemistry, sequencing techniques knowledge	No	Yes	-	Transcriptomic skills, Visualise small dataset	S1,S2,S3,S4,S5,S6

41 skills (5 fields each)

Code	Description	Level	Persona	Dependency	Training
S1	Programming in R	Basic	P1,P8	-	T1
S2	Data visualisation (in R)	Basic	P1,P7,P8,P12	S1	T4
S3	FAIR -> Software focused / Git	Basic	P12,P18	S15	T28,T32,T33,T36
S4	Data cleaning (with bash)	Basic	P1,P2,P5	-	-
S5	Transcriptomics theory	Basic	P1,P2	-	T54

55 training courses (14 fields each)

Code	Description	Link learners	Link trainers	Skill	Dependency	Easy to adopt from trainers?	Easy to adopt for learners?	Maintained?	Last update	Accept feedback?	Customizable?	Theoretical/Practical
T1	Introduction to R	https://datacarpentry.org/R-ecology-lesson/01-ir	https://github.com/data		-	Yes	Yes	Yes	2022	Yes	Yes	Practical
T2	Introduction to Python	http://swcarpentry.github.io/python-novice-gapm	https://github.com/swc		-	Yes	Yes	Yes	2022	Yes	Yes	Practical
T3	Data visualisation in Python	https://carpentries-incubator.github.io/python-int	https://github.com/carp		T2	Yes	Yes	Yes	2022	Yes	Yes	Practical
T4	Data visualisation in R	https://swcarpentry.github.io/visualization-novice	https://github.com/swc		T1	Yes	Yes	Yes	2022	Yes	Yes	Practical
T5	Orchestrating Single Cell Analysis	https://bioconductor.org/books/release/OSCA/			T1	-	-	Yes	2022	-	-	Practical
T6	Python essentials 1	https://pythoninstitute.org/python-essentials-1	-		-	No	Yes	Yes	2022	No	No	Both
T7	Introduction to R Shiny	https://shiny.rstudio.com/tutorial/written-tutorial/l	-		T1	-	-	Yes	-	-	-	-

2. Data visualization: our idea

Wet Lab

- Persona 1
- Persona 2
- Persona 3

Comput Biol

- Persona 4
- Persona 5
- Persona 6

Other

- Persona 7
- Persona 8
- Persona 9

2. Data visualization: our idea

Wet Lab
- Persona 1
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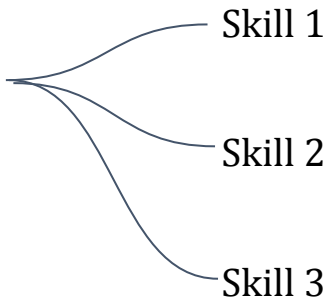
- Persona 6

Other
- Persona 7
- Persona 8
- Persona 9



Download

metadata 1
metadata 2
metadata 3
…

(for Persona 2)

2. Data visualization: our idea

Wet Lab
- Persona 1
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Comput Biol
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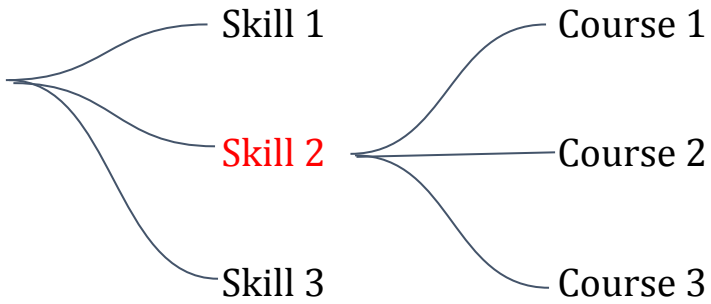

Download

metadata 1
metadata 2
metadata 3
…

(for Skill 2)

2. Data visualization: our idea

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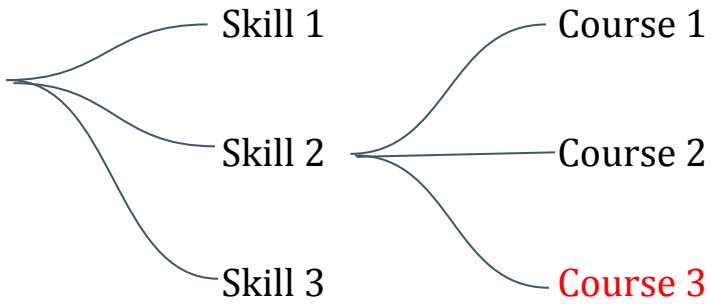


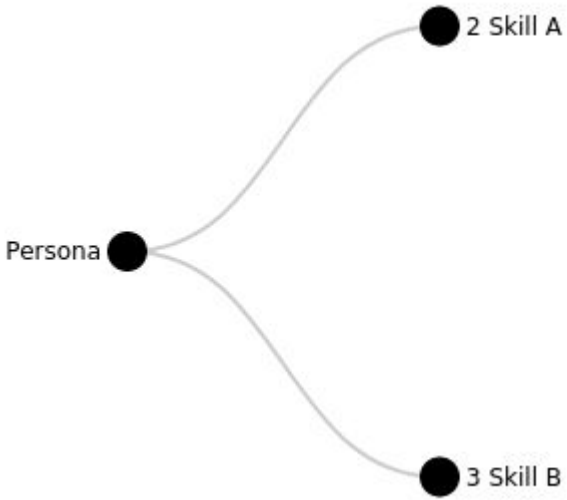
Download

metadata 1
metadata 2
metadata 3
…

(for Course 3)

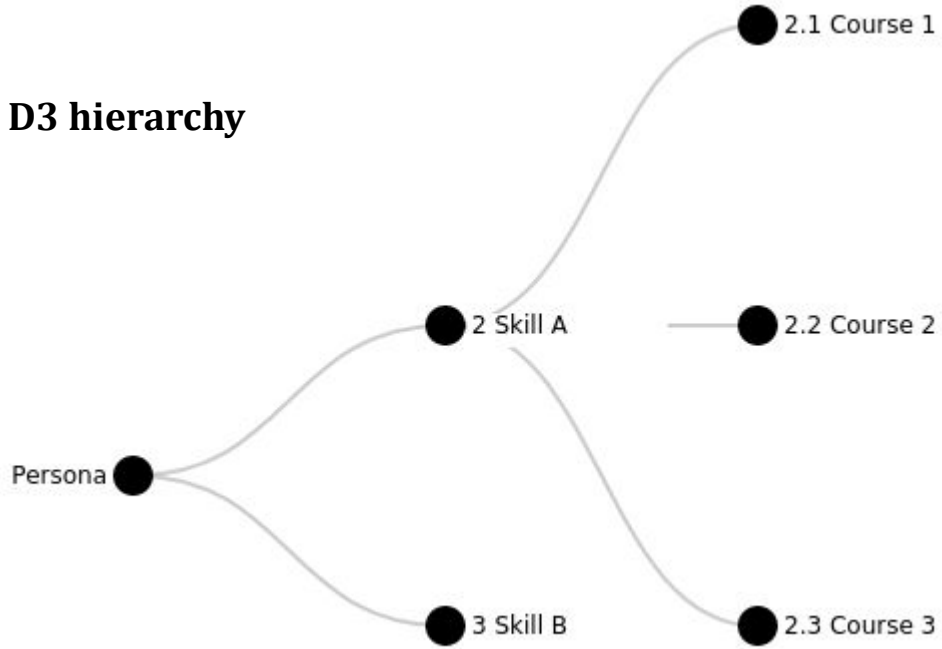
2. Data visualization: possible implementation

D3 hierarchy



2. Data visualization: possible implementation

D3 hierarchy



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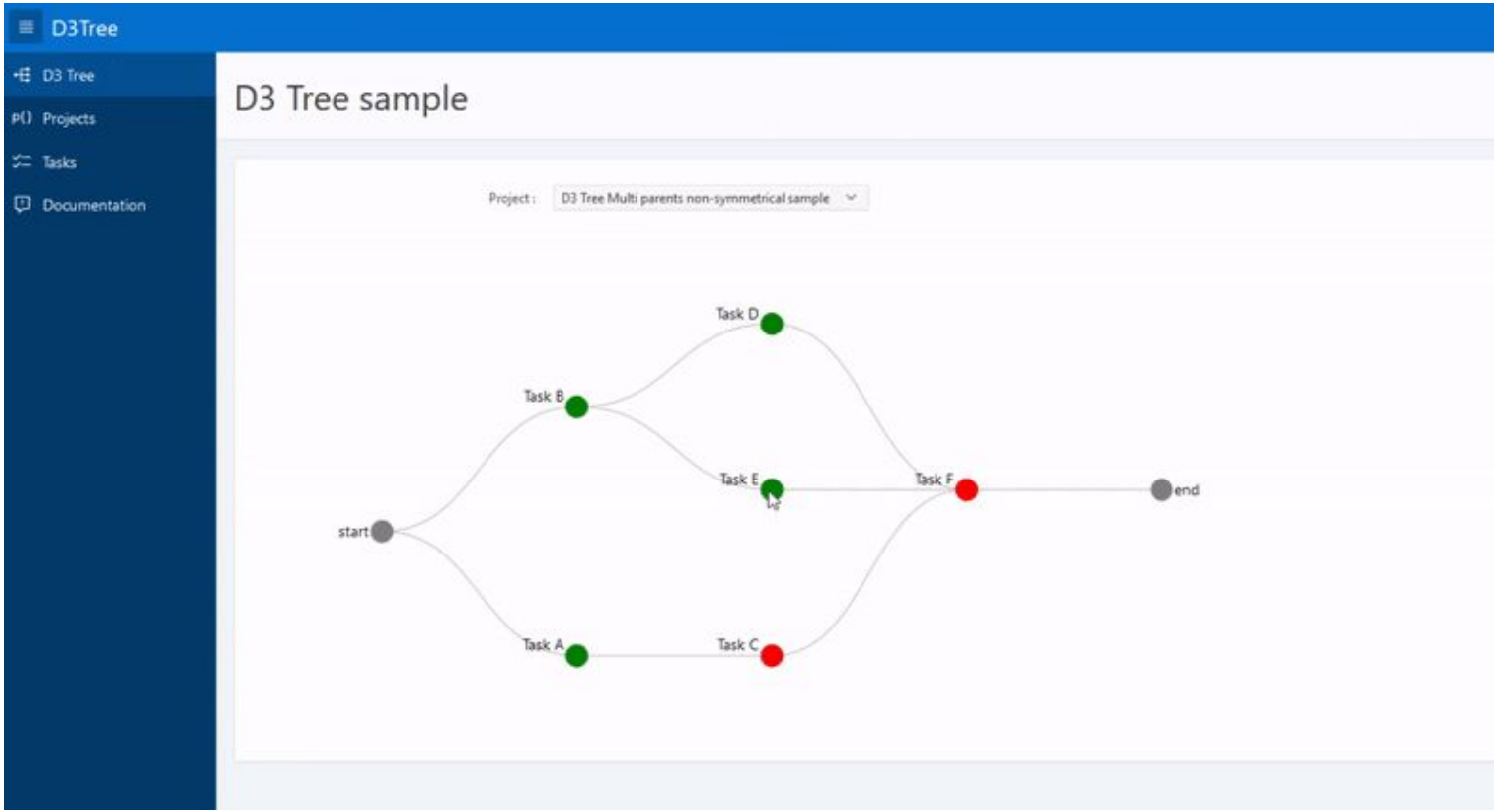
D3 hierarchy



3. Next steps

What will we do now?

Implement our data in a visual manner

What do we need?

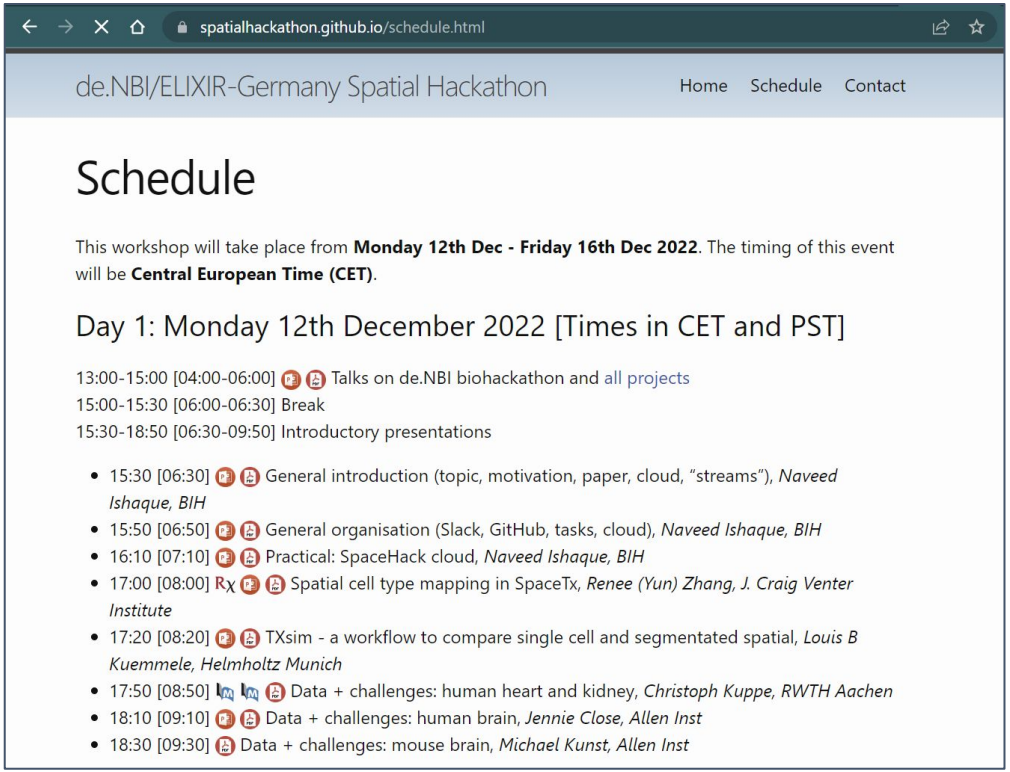
More people to expand our persona/skill/training set (currently up to ~6 people)
D3 expert(s)

Establishing best practice guidelines for imaging-based spatially resolved transcriptomics data

Naveed Ishaque (Berlin Institute of Health at the Charité) and Louis Kümmerle (Helmholtz Center München)

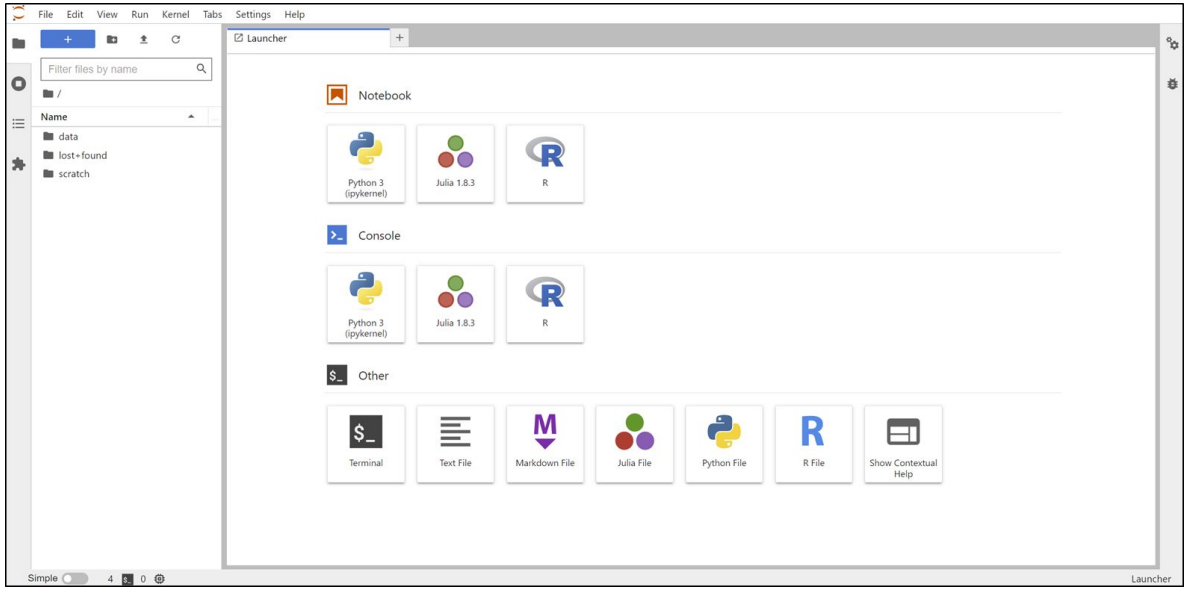
Day 1 - on boarding and motivation

- 3 introductory talks
- 2 technical methods talks
- 3 biology talks
- **Intro to `TXsim`**



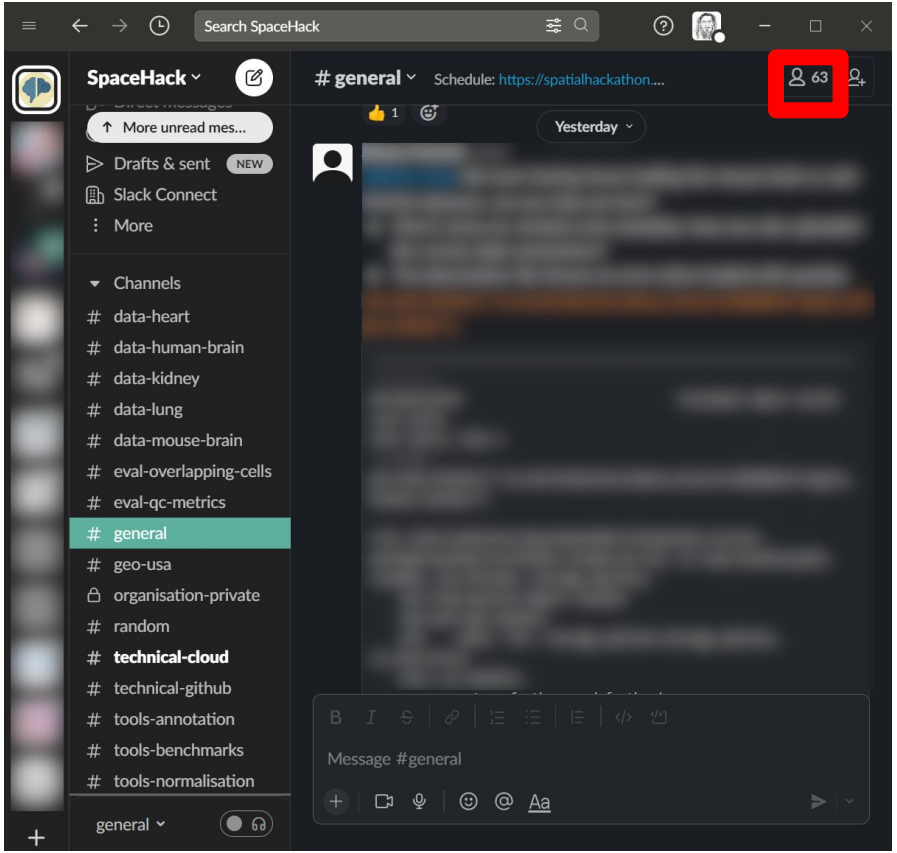
Day 2 - starting with de.NBI cloud

- ~2000 cores
- ~8 Tb RAM
- 50 Tb storage
- JupyterHub with GitHub authentication
- 2 HowTo seminars



Where we stand

- 63 participants
- 9 GitHub Repos
- 29 Slack channels
- 7 sub-projects



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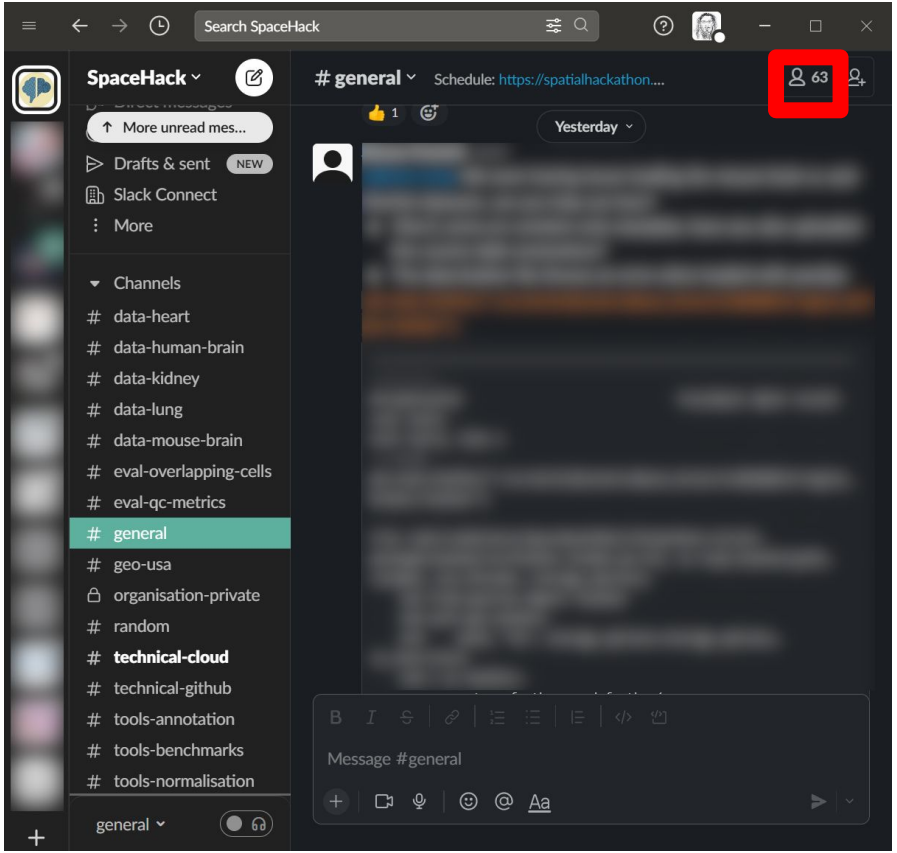
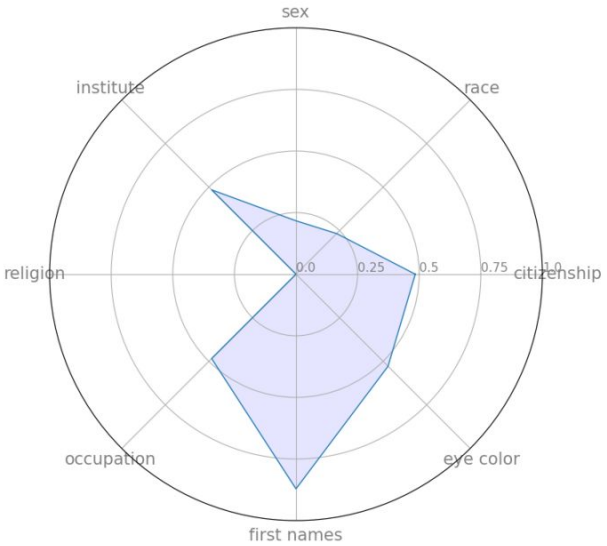


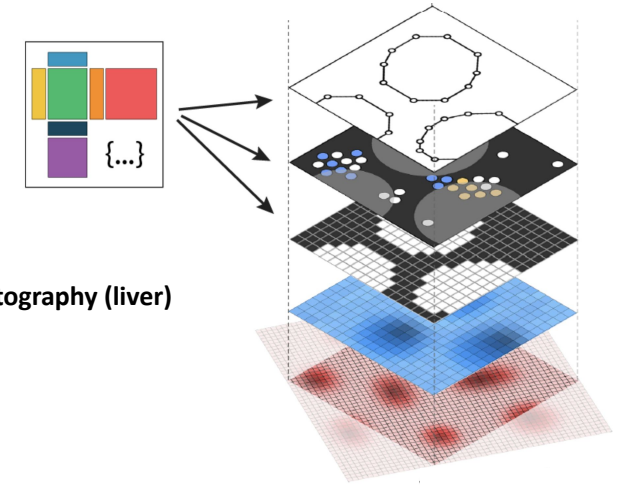
Project 1: #xenium_omni_pipeline

- **Project motivation:** Evaluation of added value of Xenium technology and designing the analysis workflow
- **Our solution**
  - Creating necessary infrastructure using `SpatialData` & `TXsim`
  - QC of the workflow
  - Multiomics integration and analysis
- **Update points**
  - Imported Xenium & Visium into `SpatialData` format, napari-assisted registration
  - `Napari` plugin for smooth histopathological annotation
  - Xenium & scFFPE annotated
  - Visium & scRNA-seq copy number projection
  - Diversity plot of the group created



Project 2: #zarr_for_data_and_metadata

- **Project motivation**
  - Analyzing multiple spatial datasets with all their metadata takes a **long time and varies in quality**
- **Our solution**
  - Increase **interoperability and performance** using a new standard: `SpatialData`
  - Add metadata for **physical distances**
    - useful for upcoming methods like Project 4: finding overlapping cells in z-dimension
  - Document and make **reproducible** using `spatial-sandbox`
- **Updates**
  - `SpatialData` with physical coordinates done for **Xenium (breast) and Molecular Cartography (liver)**
  - Documentation of the physical distance metadata sometimes **not there or hard to find**
  - WIP: lung (Wouter-Michiel), mouse brain (Luca), heart (Benjamin)

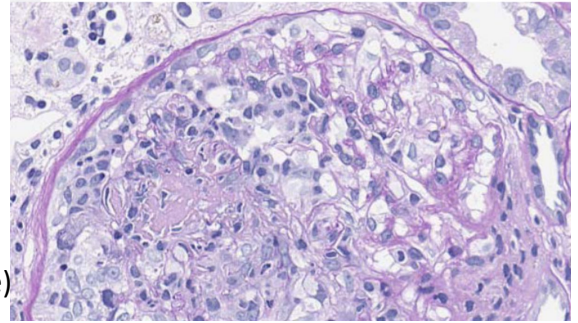


Project 3: #segmentation-x

- **Project motivation**

  How do we segment the un-segmentable?
  Deep learning / expert annotation / membrane stains / segmentation-free?

  Optimize parameters and setup pipelines



- **Current tasks we are working on**

Florian Wuennemann
FloWuenne

`SSAM` + `Baysor` on transcripts from human heart MERFISH data (Kuppe)

Sebastian Gonzalez Tirado
sebgoti

Large scale data segmentation with Cellpose 2.0
(heart/in_situ_sequencing/human-in-the-loop approach)

Valentina Beliaeva
Kraftfahrzeughaftpflichtversicherung

Airat Valiev
Rebell-Leader

Liya Zaygerman
theinvisibleliya

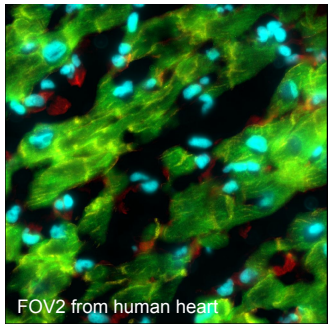
Sebastian Zürner
zu-se

Testing mesmer with membrane stains on heart data
+ Include `Mesmer` and `JSTA` in `TXSim`

pakiessling

Christoph Kuppe
chkuppe

Testing `Cellpose2` on Kuppe data (human-in-the-loop retraining)



Project 4: #eval-overlapping-cells

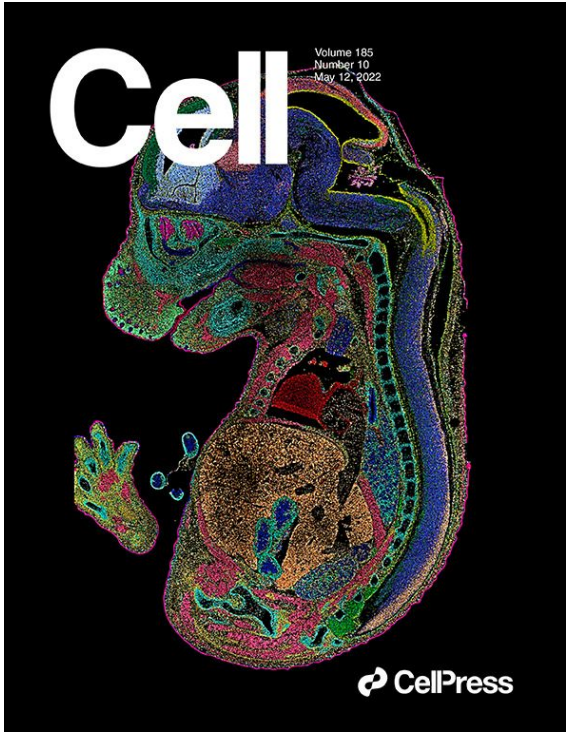
- **Project motivation**: Overlapping cells cause problems in analysing spatial gene expression.
- **Our solution:** Utilise Z-plane information to find cells that overlapping
- **Updates**
  - Adapting a script to make it work on our different data sets
  - Script close to done, 1st data set analyzed
  - Working on visualization automatization

Project 5: #brain-evaluation

- **Project motivation**: quantitative and qualitative interpretation on quality metrics for single-cell vs spatial gene expression is not trivial due to lack of general understanding of these metrics
- **Our solution:**
  - Evaluate single cells of the brain tissue of mouse and/or human
  - Create vignettes for metric measures in the `TXsim` pipeline.
- **Updates**
  - Run the `TXsim` pipeline on test dataset:
    - Resolution differences between `watershed` vs `cellpose`
    - Single cell type annotation in the spatial context
    - Modify cell sizes based on type
  - Understanding metric scripts, trying different parameters and running on test datasets.

Project 6: #stereoseq

- **Project motivation - what is the problem?**
  - Stereoseq is a new and exciting spatial technology!
  - Currently not supported in our TXsim workflow
- **Our Solution**
  - **Stereo-seq**: [Xia et al. 2022] [Chen et al. 2022]
  - Enables cell type and cell-subtype characterization and profiling based on both transcriptome and spatial information.
  - Integrate different segmentation tools (eg:`ssam`, `msmer`) to work with full transcriptome data
- **Updates**
  - Data Compilation and software setup
  - Troubleshooting
  - Initial sanity checks of the input data-set



Project 7: #hyperbolic_brain

- **Project motivation - what is the problem?**
  - The cell type segmentation and annotation process can still be improved
- **Our solution**
  - Applying hyperbolic space embedding and distance metrics as an alternative to the classical euclidean-based segmentation and annotation pipeline
- **Updates**
  - Obtained Xenium Human Brain tissue dataset and applied a simple `squidpy` analysis and visualization process
  - Started the algorithm to embed the transcript levels data to hyperbolic space

Summary

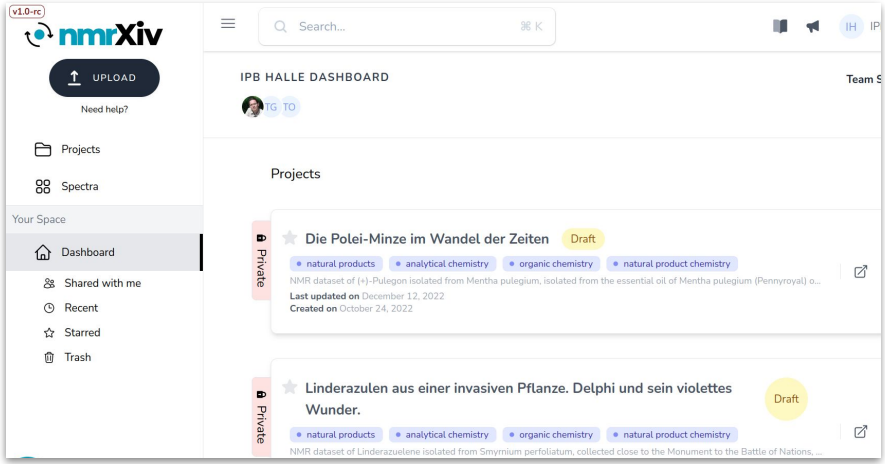
- A hackathon project with 63 participants present certain challenges
  - Despite all issues, things have fallen into place
  - Integrating online participants isn’t easy (sorry!)

(Bio)Schemas4NFDI, lightweight domain metadata (not only) for NFDI consortia

Steffen Neumann (IPB Halle) and Leyla Jael Castro (ZB MED)

Data Provider Department

nmrXiv



Achievements:

- Describe nmrXiv as `DataCatalog`
- `Sample` -> `BioSample`
- Improve `MeasurementTechnique` & `keywords`

HELP !!

Fix Bioschemas validator
ElixirTeSS/bioschemas-validator
Fix keywords as definedTerm

Data Provider Department

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN

QBiC

- Sequencing platform
- Proteomics platform
- Metabolomics platform
- Imaging platform

produce

annotated
datasets + studies

??

~ 10,000 datasets / year

Google
Dataset
Search

OmicsDI

access

web portal

Achievement: 1st Bioschemas crosswalk and model draft

Lesson learned: Google Dataset Search only cares for `Dataset`, `DataCatalog` and `DataDownload`

Crosswalking Department

"For models defined in LinkML, what is the best way to export dataset metadata into Bioschemas JSON-LD for inclusion in data provider pages."

Achievements:

- Dataset crosswalk spreadsheet between GHGA's metadata YAML & Bioschemas
- Added "exact_mapping" elements to a hackathon copy of ghga.yaml
- Developed prototype LinkML code for the translation from YAML to JSON-LD

Lessons learned:

- LinkML maintainer(s) have raised the point that the original crosswalk.yaml may not be sufficient for a common solution.

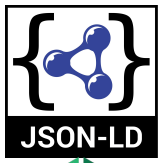
Querying / Harvesting Department

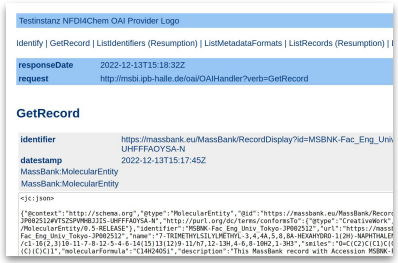
Chemotion

MassBank
High Quality Mass Spectral Database

nmrXiv

OAI-PMH





HELP !!
~~python xtree~~
~~xpath and~~
~~namespaces~~

NFDI4C

ckan

Achievements:

- MassBank in OAI-PMH
- Harvesting bioschemas through OAI-PMH

Google Dataset Search

Lessons learned:

- Only indexing `DataSet`
- Re-indexing needs `Last-changed-date`

Towards FAIR Computational Metabolomics Workflows - Improving Provenance Collection

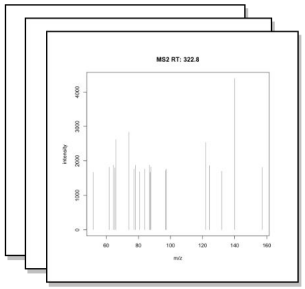
Mahnoor Zulfiqar (University of Jena)
Kristian Peters (IPB Halle)
Michael R. Crusoe (ELIXIR-DE)

Example Workflow

Metabolome Annotation Workflow

https://github.com/zmahnoor14/MAW

Input



MAW-R

Output

Result Folders

Input

Result Folders

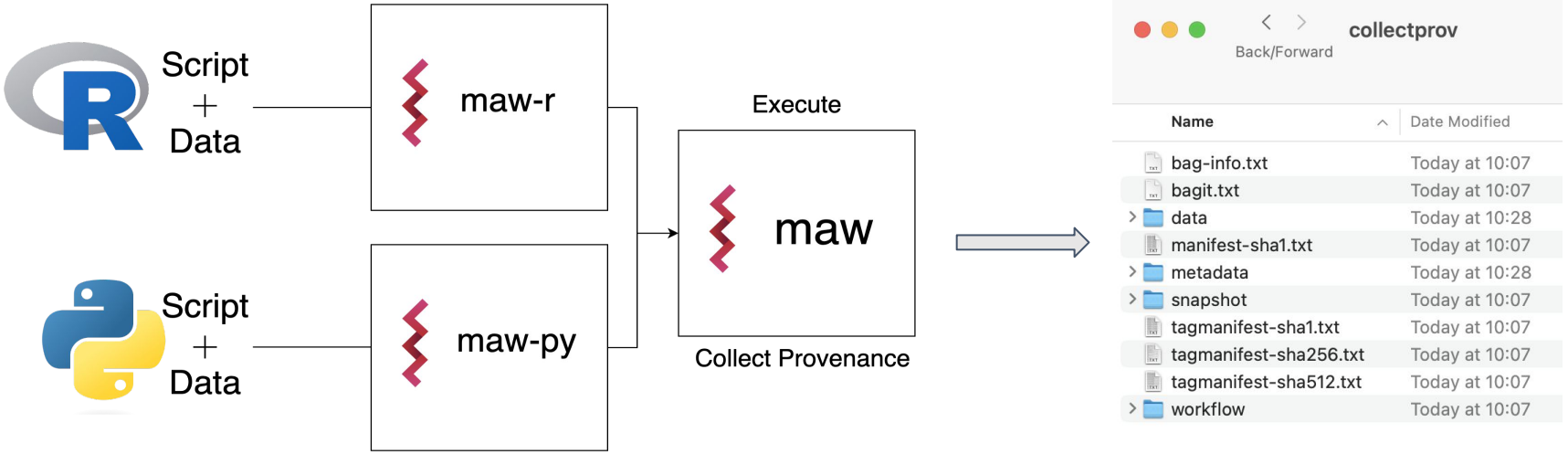
MAW-Py

Output

Feat	m/z	rt	Nan	SMI	Form	M	Sour	Class
ID1	379.	102.	Prol	C1C(	C_5H_9	2	GN Suspe	Amin acids
ID2	244.	356.	Phos 3-su	C([C	C_3H_3	3	PubC	Phosp este
...								
ID4	350.	276.	NA	NA	$C_{13}H_$	4	SIRI Form	Pur nuclec

Progress

- Goals achieved:
  - Wrote CWL CommandLineTool descriptions for the R step and the Python step
  - Combined those steps into a CWL workflow MAW
  - Upgraded the Docker container for the R step to not need to be run interactively; rebuilt for linux/amd64
  - Collected workflow execution provenance using CWLprov



Goals

- Further goals
  - Convert the CWLProv RO-Bundle to a Workflow Run RO-Crate using runcrate
  - Add annotations using the EDAM ontology
  - Generate provenance of the separate analysis steps with the R step and the Python step; explore how to pass that information to CWLProv/RO-Crate
  - Run the workflow using toil-cwl-runner on the ARA Slurm cluster

Find us here:

SR 8 (2nd floor)
Slack channel: #fair-workflow

Interactive data analysis and visualization in the web browser

Asis Hallab (FZ Jülich) and Ata Ul Haleem (FZ Jülich)

Project turns out to be an ugly wallflower

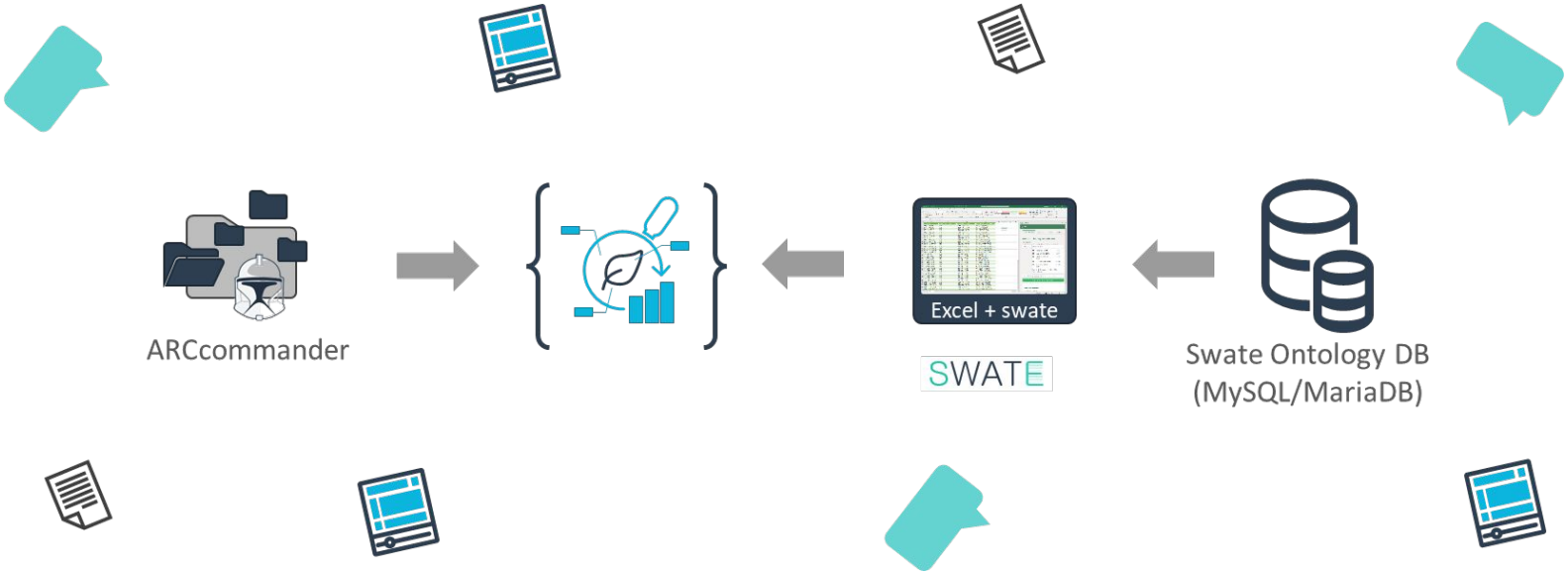
No advances made;
we are sorry.

But hey,
my luggage arrived and
my co-lead's son is getting better..

DataPLANT - Facilitating Research Data Management to combat the reproducibility crisis

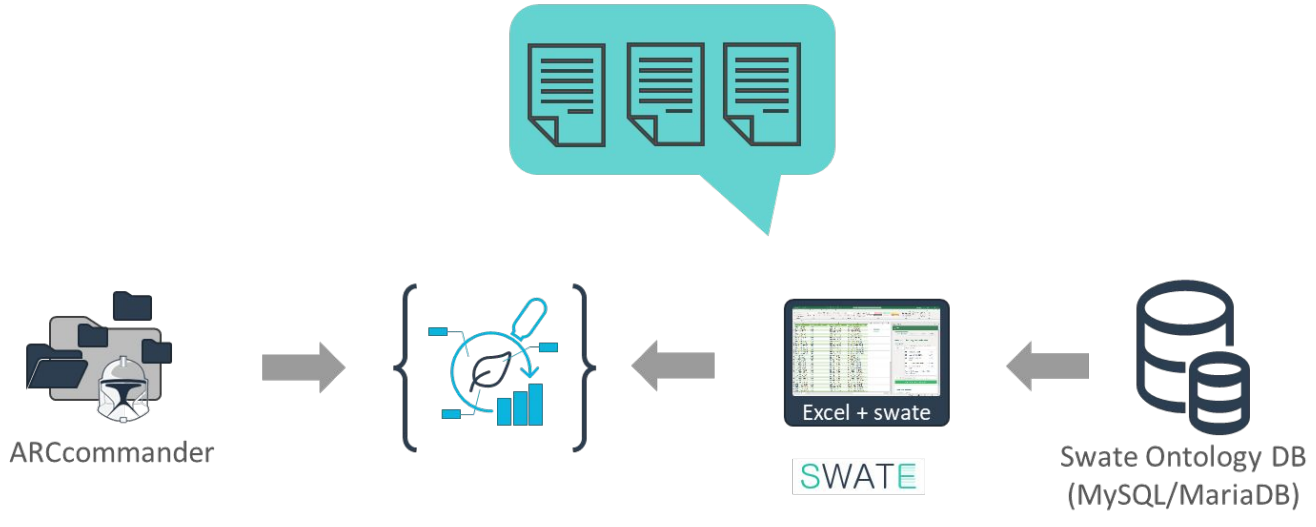
Elisa Senger (FZ Jülich) and Lukas Weil (TU Kaiserslautern)

Centralization of training materials



Centralization of training materials

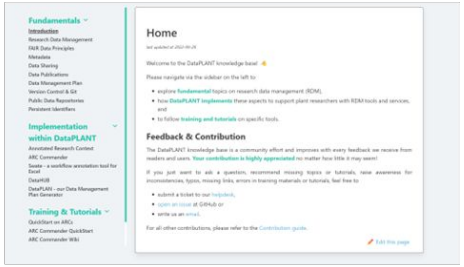
Centralized KnowledgeBase with tutorials for consumers



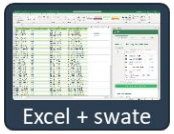
Tool specific Documentation for developers and data stewards

Centralization of training materials

Centralized KnowledgeBase with tutorials for consumers

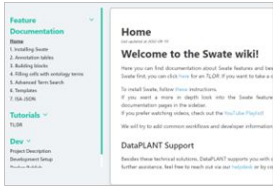


ARCcommander



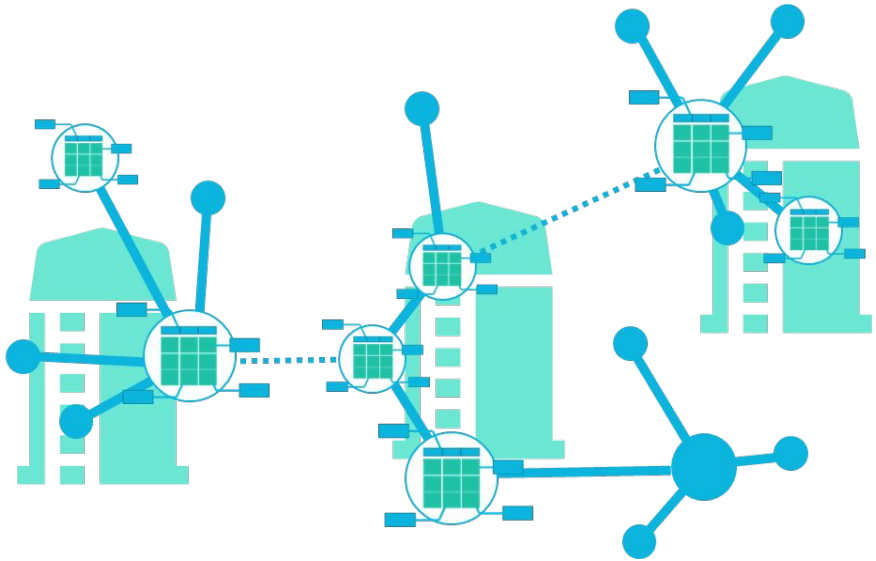
SWATE

Swate Ontology DB
(MySQL/MariaDB)

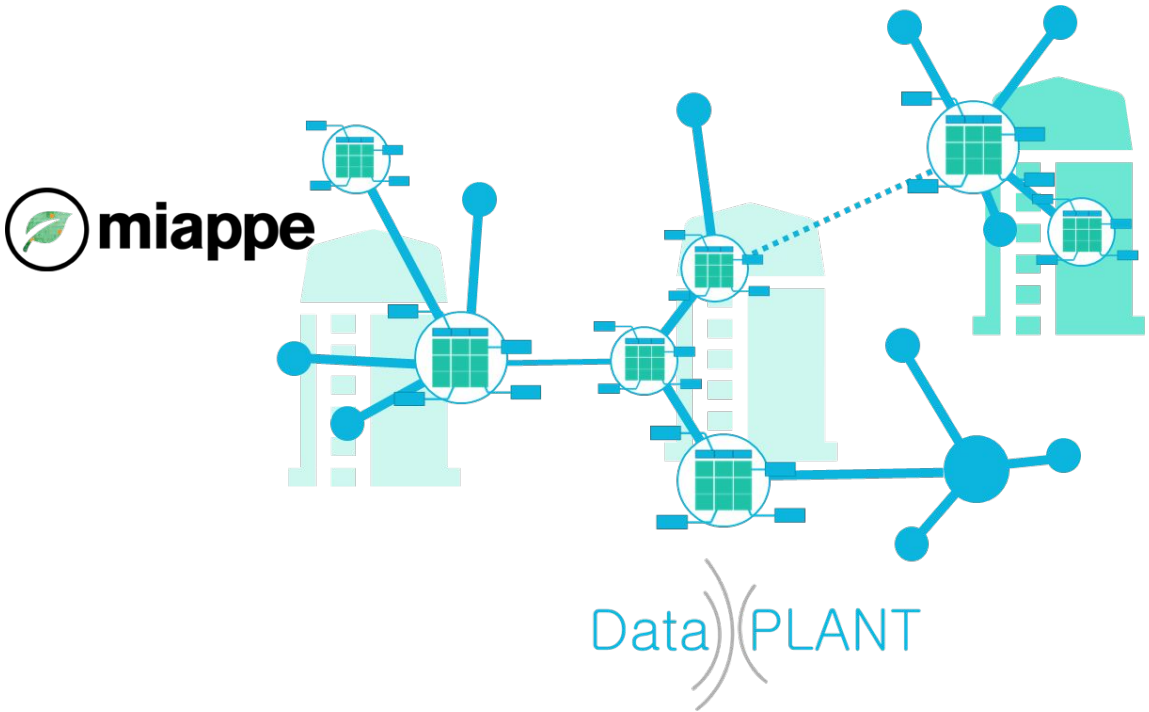


Tool specific Documentation for developers and data stewards

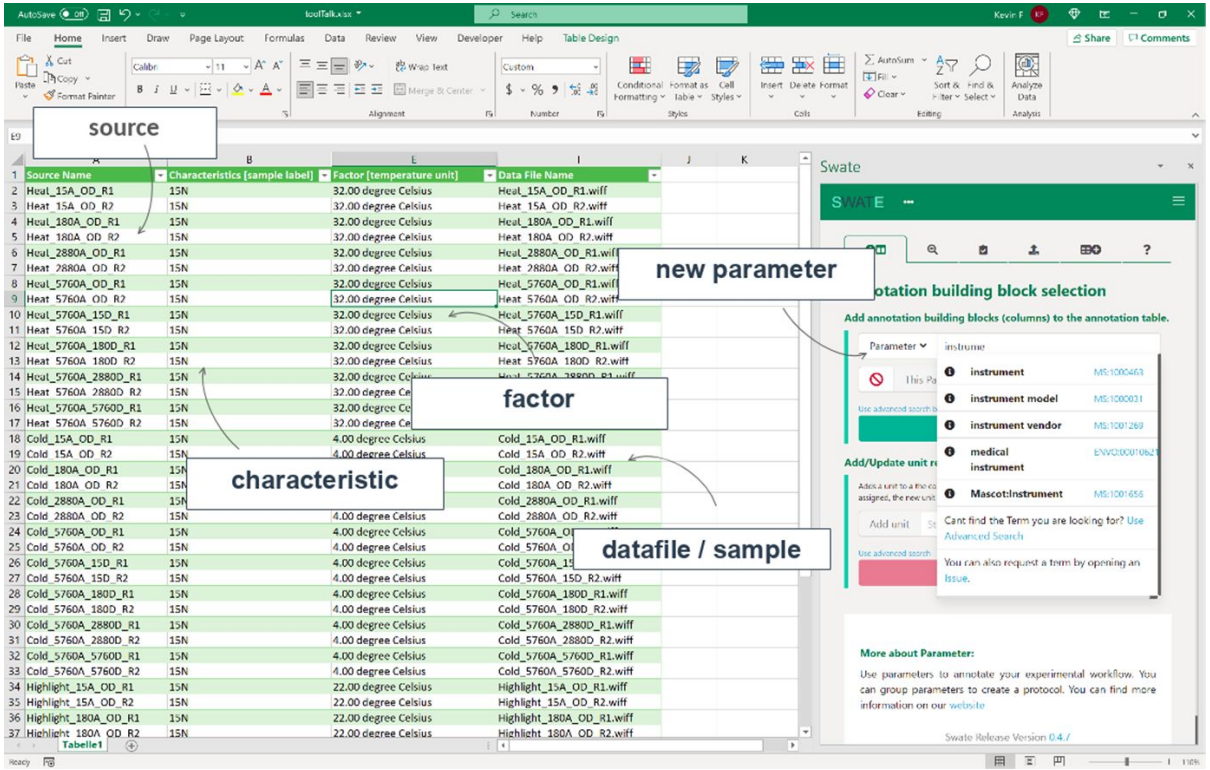
Creating a MIAPPE template



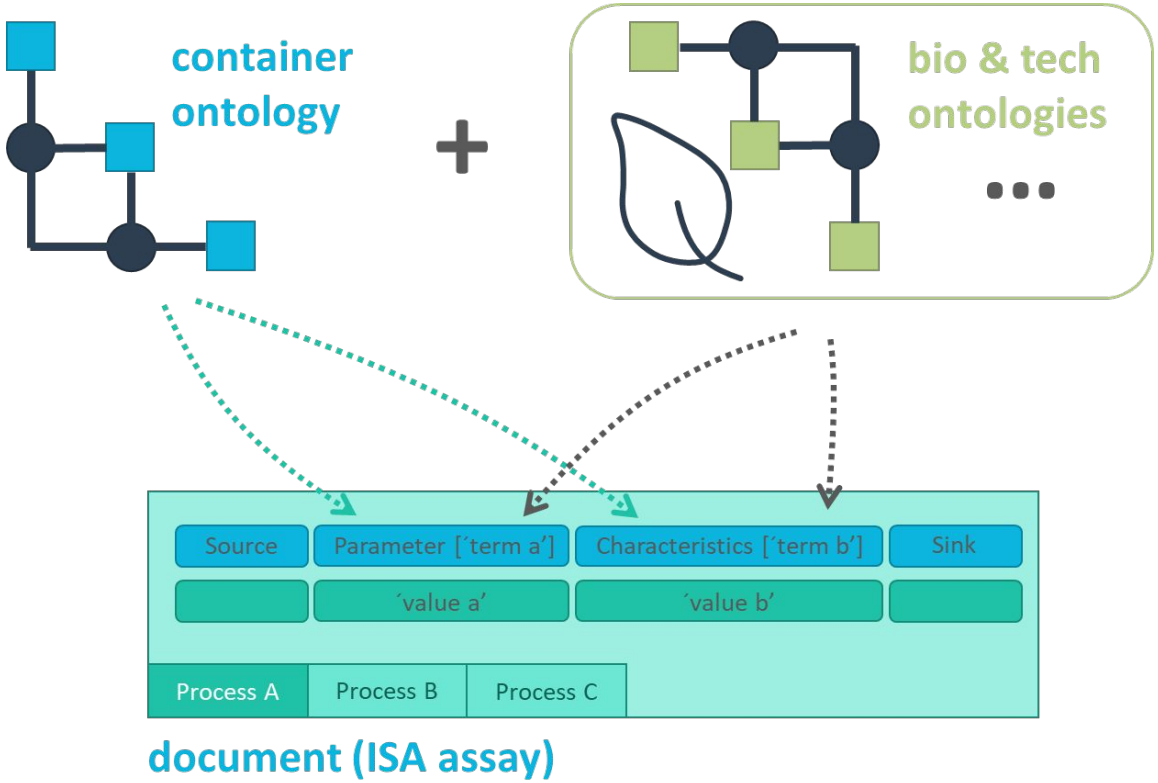
Creating a MIAPPE template



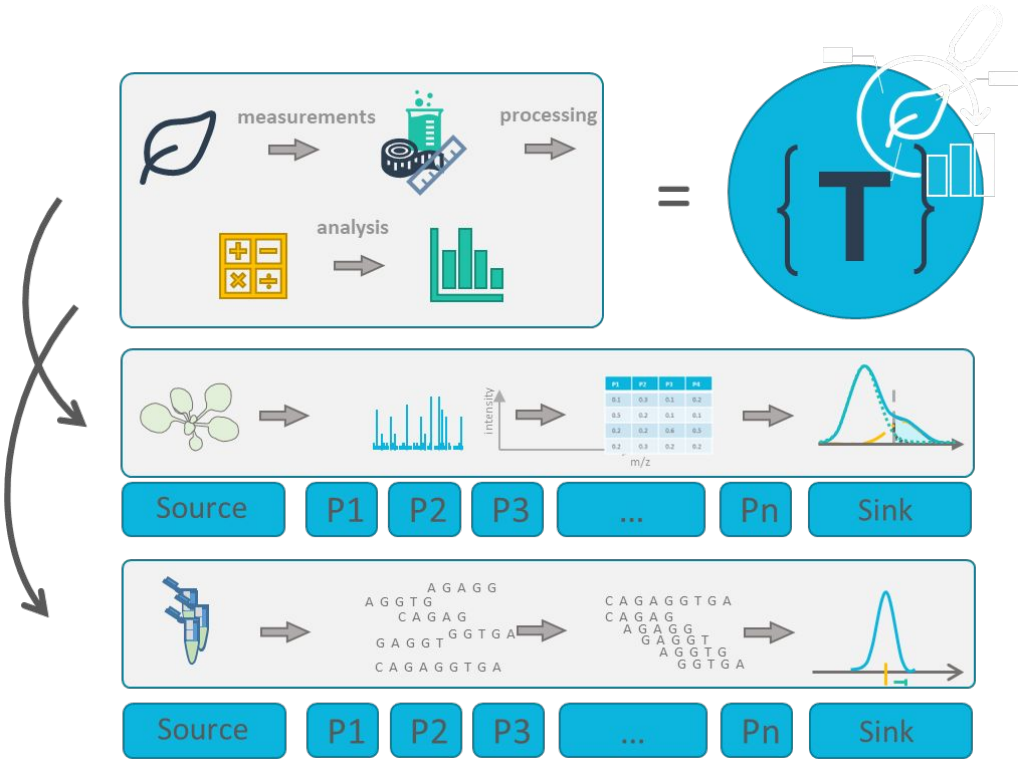
Creating a MIAPPE template



Creating a MIAPPE template



Creating a MIAPPE template



Creating a MIAPPE template

Swate

Building Blocks

Add annotation building blocks (columns) to the annotation table.

Parameter | experiment start

Experiment Start Date NCIT:C90487

Definition: "The date on which an experiment begins." []

Experiment NCIT:C42790

experiment name MS:1002120

Experiment Name NCIT:C181729

experiment performer EFO:0000647

Cant find the Term you are looking for? Try Advanced Search!

Still can't find what you need? Get in contact with us!

More about Parameter:

Ontobee

Home | Intro | Statistics | SPARQL | Ontobeep | Annotator | Tutorial | FAQs | Ref

Please select an ontology (optional)

Keywords: experiment start date | Search terms | Batch Search

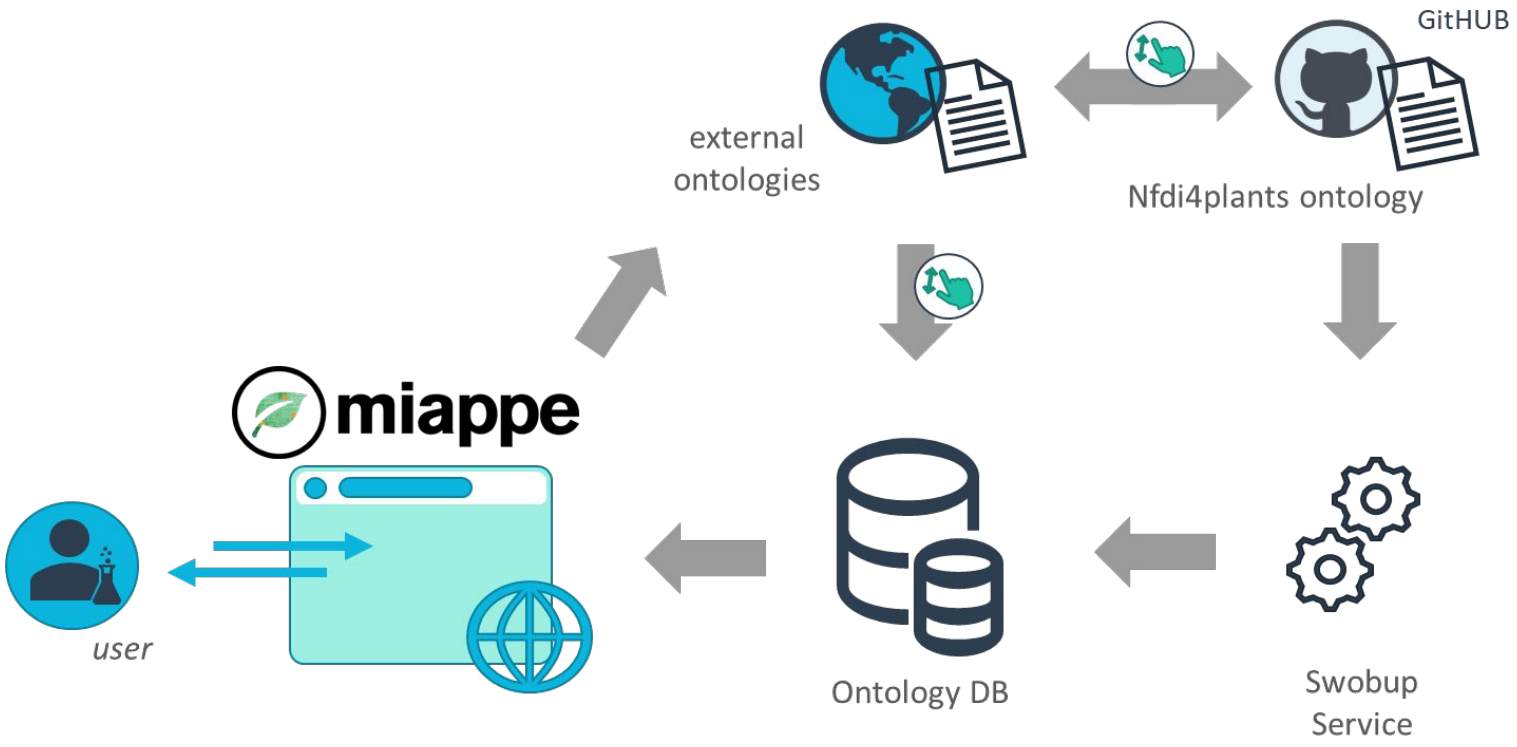
Terms with 'experiment start date' included in their label:

1. http://purl.obolibrary.org/obo/NCIT_C90487 **(NCIT)**:
   - **Experiment Start Date** *in Ontobee*: NCIT
2. http://purl.obolibrary.org/obo/AGRO_00000684 **(AGRO)**:
   - **experiment start date** *in Ontobee*: AGRO

B	E	H
Parameter [MIAPPE version]	Parameter [Experiment Start Date]	Parameter [Experiment End Date]
The version of MIAPPE used.	Date and, if relevant, time when the expe	Date and, if relevant, time when the exp
1.1	2002-04-04 2006-09-27T10:23:21+00:00	27.11.2002
Version number	Date/Time (ISO 8601, optional time zone	Date/Time (ISO 8601, optional time zon
1	1	0-1

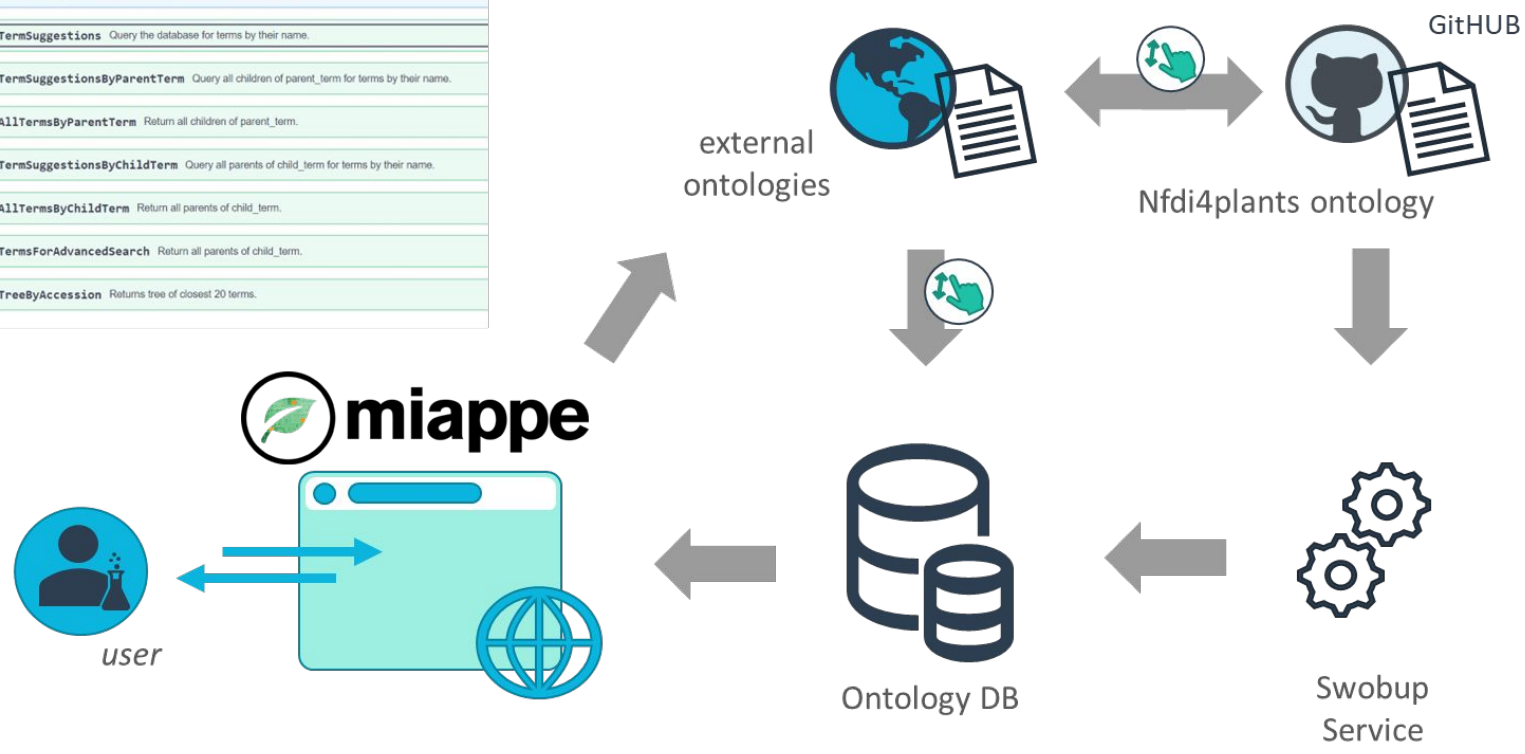
A	D	G
Characteristic [Rooting medium]	Characteristic [Container type]	Characteristic [Container volume]
An abiotic plant treatment (EO:000719	Type of container used to grow/treat	Volume that is available to the roots. XE
hydroponic plant culture media; in vitro	pot; Petri dish; well; tray	[L]
Plant Environment Ontology:'EO_0007	Text	Numeric

DataPlant Ontology Service

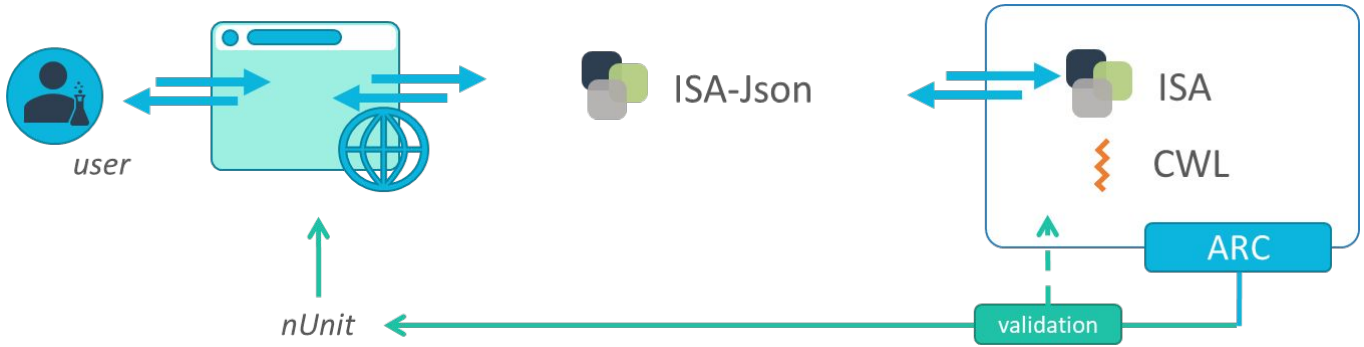


DataPlant Ontology Service

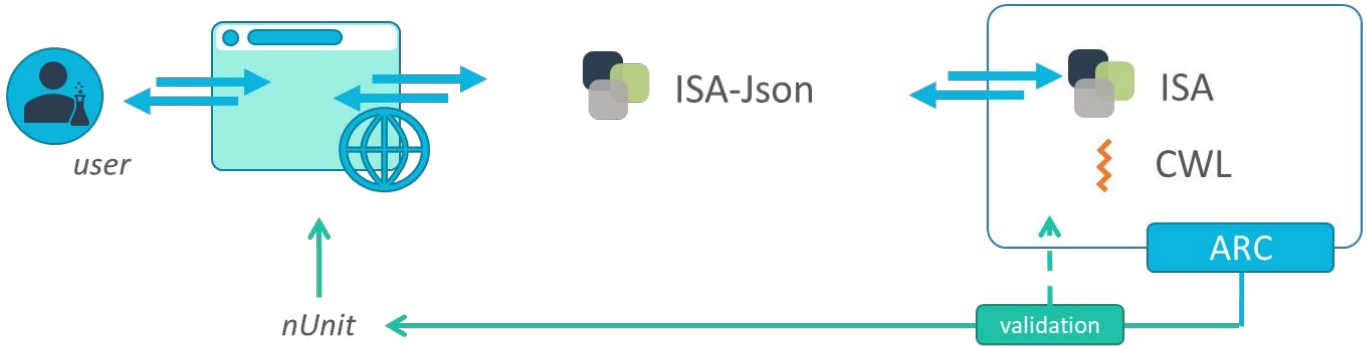
GET	/api/IOntologyAPIv2/getTestNumber	Test function to verify client server connection.
GET	/api/IOntologyAPIv2/getAllOntologies	Returns all ontologies found in the database.
POST	/api/IOntologyAPIv2/getTermSuggestions	Query the database for terms by their name.
POST	/api/IOntologyAPIv2/getTermSuggestionsByParentTerm	Query all children of parent_term for terms by their name.
POST	/api/IOntologyAPIv2/getAllTermsByParentTerm	Return all children of parent_term.
POST	/api/IOntologyAPIv2/getTermSuggestionsByChildTerm	Query all parents of child_term for terms by their name.
POST	/api/IOntologyAPIv2/getAllTermsByChildTerm	Return all parents of child_term.
POST	/api/IOntologyAPIv2/getTermsForAdvancedSearch	Return all parents of child_term.
POST	/api/IOntologyAPIv2/getTreeByAccession	Returns tree of closest 20 terms.

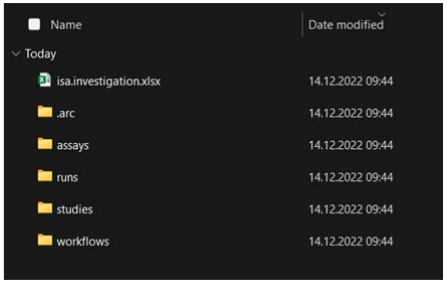


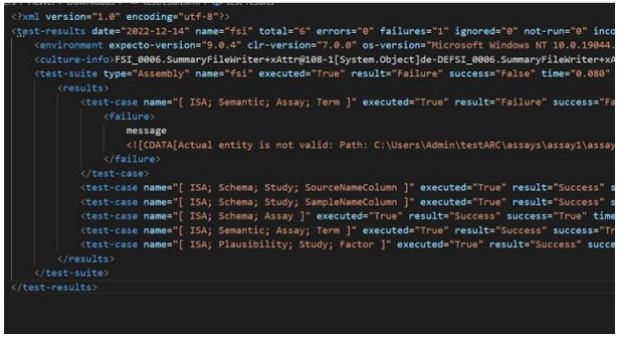
Centralized interfaces



Centralized interfaces







	A	B	C	D	E	F
1	Source Na	Paramete	Term Sou	Term Acc	Paramete	Unit
2	run_35_A	control	EFO	http://purl.ol	25	degree Celsiu
3	run_35_B	control	EFO	http://purl.ol	25	degree Celsiu
4	run_35_C	control	EFO	http://purl.ol	25	degree Celsiu
5	run_40_A	control	EFO	http://purl.ol	25	degree Celsiu
6	run_40_B	control	EFO	http://purl.ol	25	degree Celsiu
7	run_40_C	control	EFO	http://purl.ol	25	degree Celsiu
8	run_35_A	control	EFO	http://purl.ol	25	degree Celsiu
9	run_35_B	control	EFO	http://purl.ol	25	degree Celsiu
10	run_35_C	control	EFO	http://purl.ol	25	degree Celsiu
11	run_40_A	control	EFO	http://purl.ol	25	degree Celsiu
12	run_40_B	control	EFO	http://purl.ol	25	degree Celsiu
13	run_40_C	control	EFO	http://purl.ol	25	degree Celsiu
14	run_35_A	treatment	OGMS	http://purl.ol	35	degree Celsiu
15	run_35_B	treatment	OGMS	http://purl.ol	35	degree Celsiu
16	run_35_C	treatment	OGMS	http://purl.ol	35	degree Celsiu
17	run_35_A	treatment	OGMS	http://purl.ol	35	degree Celsiu
18	run_35_B	treatment	OGMS	http://purl.ol	35	degree Celsiu
19	run_35_C	treatment	OGMS	http://purl.ol	35	degree Celsiu
20	run_35_A	treatment	OGMS	http://purl.ol	35	degree Celsiu
21	run_35_B	treatment	OGMS	http://purl.ol	35	degree Celsiu

The ELIXIR::GA4GH Cloud

Mohsen Pourjam (TUM)
Alexander Kanitz (ELIXIR-CH)

Project: Solve use case for TUM

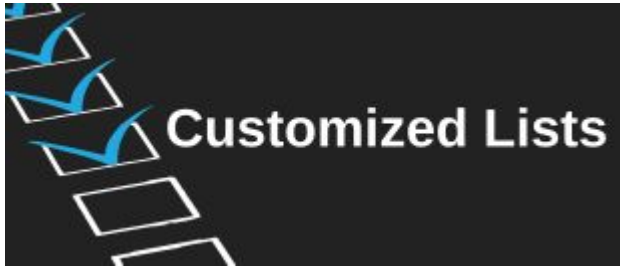
- Pipeline to **process** 16S rRNA gene sequences
- Deciphering **microbial composition** from 16S rRNA

What if we could enrich our hypothesis with datasets acquired with the same hypotheses?

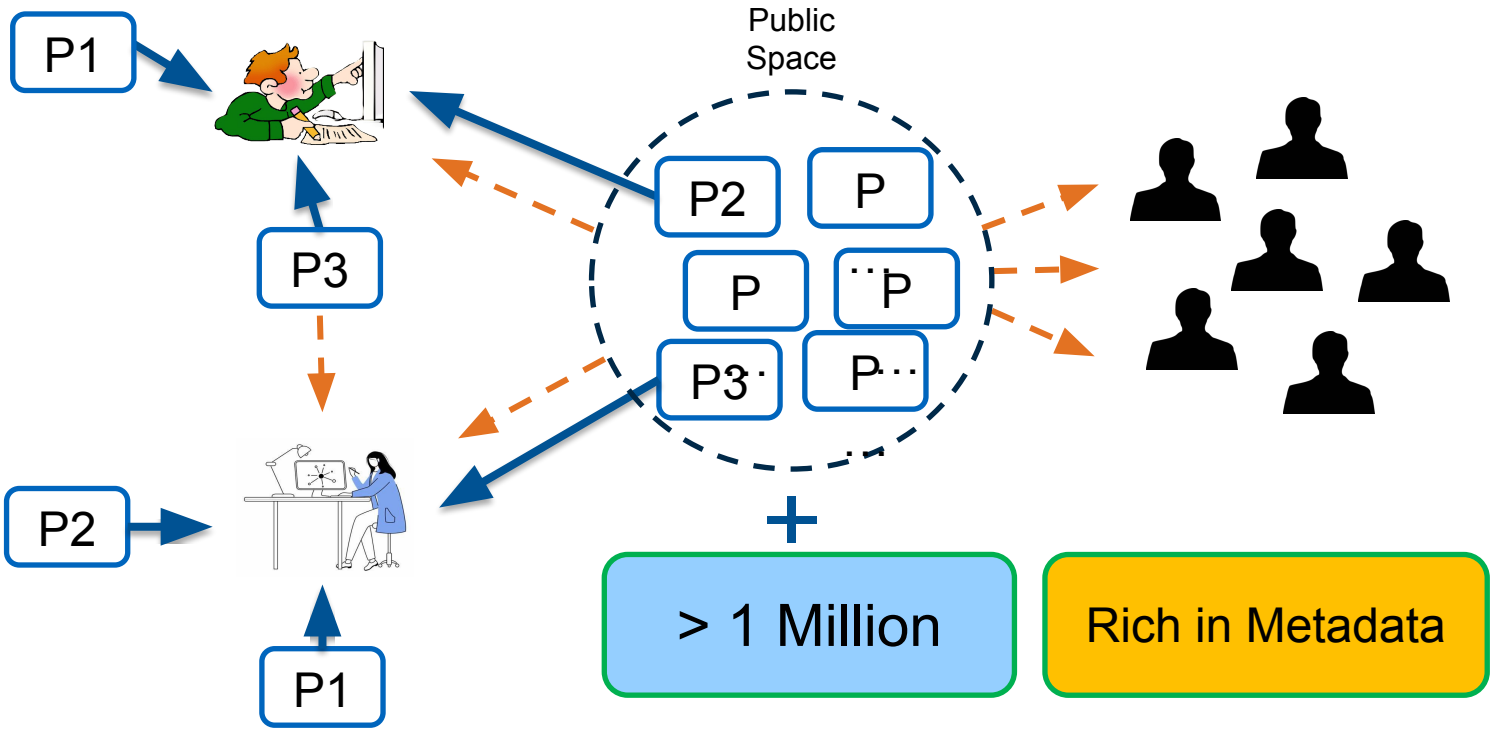
- How can I **find** datasets produced to address the similar hypothesis?
- How can I **process** my data as well as other projects data?
- Would my results be **comparable** to other projects results?
- How can I **store** it with relevant metadata?
- How can I **share** or use shared data?

What does IMNGS2 provide?

www.imngs2.org



IMNGS2:


P1
P3
P2
P1
Public Space
P2
P
P
P
P3
P
+
> 1 Million
Rich in Metadata
All Environments

Where is the problem?

- 3 min * 1,050,000 ≈ 6 years
- The solution is **parallelization**
- Still the problem is there ⟹ lack of infrastructure
- An unsuccessful try with ELIXIR Greece

Migrate to workflow language

Why?

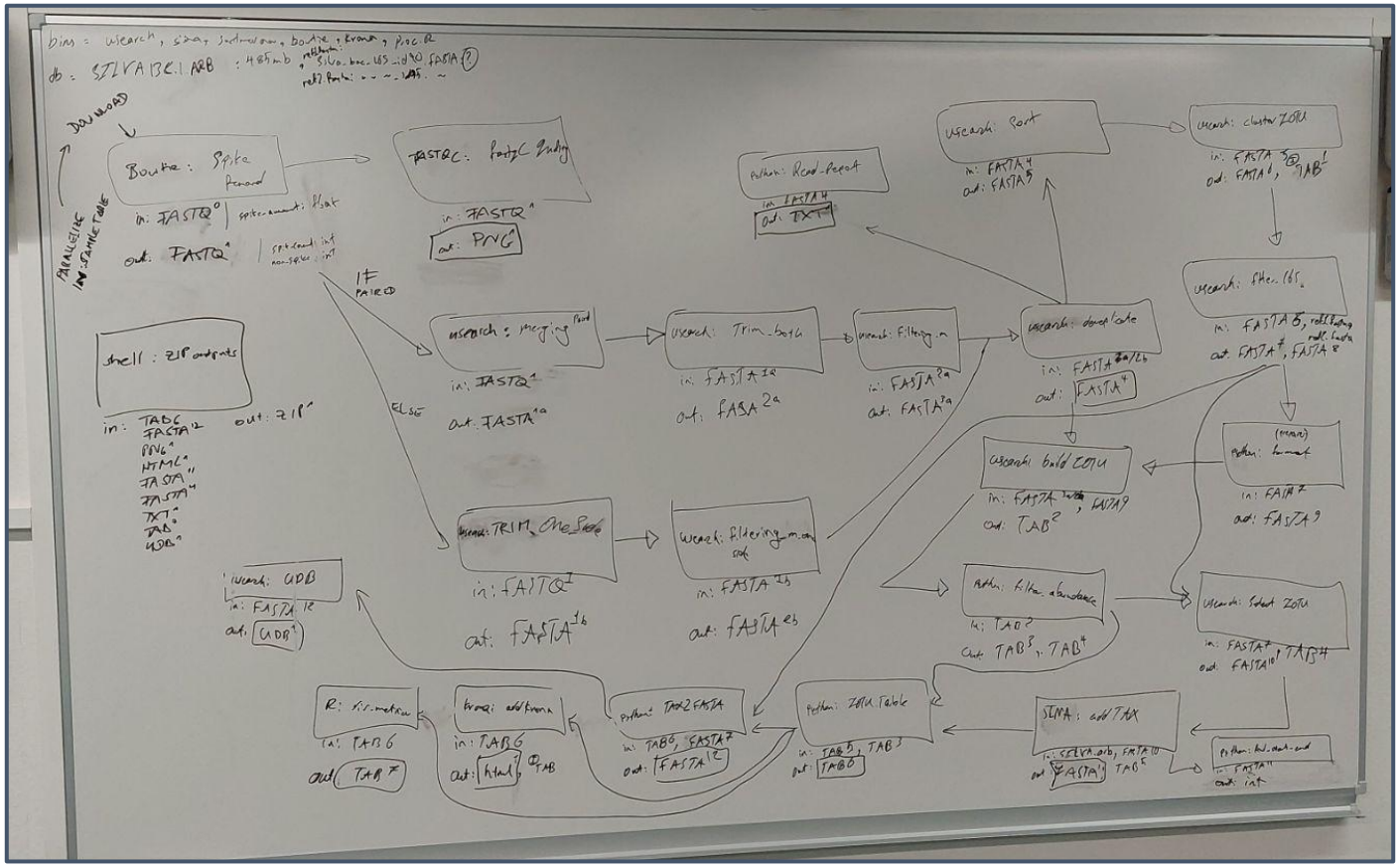
- Better for parallelization / horizontal scaling
- Resource provisioning per step allows optimizing resource use (highly relevant for >1 million jobs)
- Many execution options (HPC, cloud etc.)
- Allow partial (& automatic) reruns
- More portable (containerization; easier to deploy for others)
- Easier to maintain

Use Snakemake

Why Snakemake?

- Supported by ELIXIR::GA4GH Cloud
- Has GA4GH TES backend for task-level federation
- Supported by Amazon Genomics CLI as alternative
- Easy to migrate from Python-based pipeline; custom functions can be executed +/- as is via `run` directive, no need to “scriptify”

Step 1: Manual DAG :)



Step 2: Identify container images

Containerized workflows are most portable!

- Bowtie 2: `quay.io/biocontainers/bowtie2:2.4.4--py37hafa4d4c_1` /
- Krona: `quay.io/biocontainers/krona:2.7.1--pl526_5`
- SINA: `quay.io/biocontainers/sina:1.6.0--hc7f9b0f_1`
- SortMeRNA: `quay.io/biocontainers/sortmerna:4.2.0--h9ee0642_1`
- R: `r-base:3.5.2` or `rocker/r-ver:3.5.2` (would prefer the latter, see here)
- Python: `python:3.7.16-slim-bullseye`

✓ **BioContainers or official images** available for tools* 🥳
⇒ ***Great for reproducibility!***

(Custom images may or may not be there tomorrow, next month, in 5 years)

* Well, almost all - more on that later

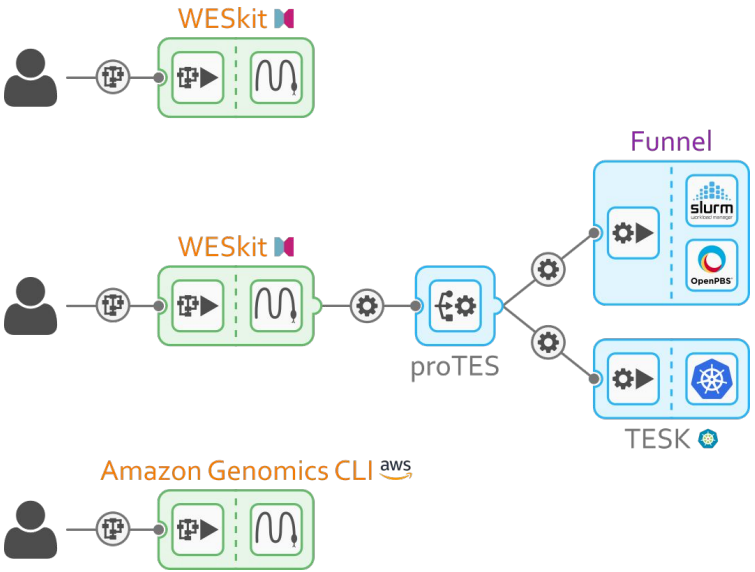
Step 3: Prepare set of test files

GERMAN NETWORK FOR BIOINFORMATICS INFRASTRUCTURE

- ✓ ***Set of input files prepared***

Next steps

- Generate Snakemake skeleton with all steps from manual DAG
- Divide up steps into individual issues
- Test execution on cloud infrastructure
    - **WESkit only**
      @ ELIXIR DE
    - **WESkit + TES backend**
      @ ELIXIR CZ/FI/GR
    - **Amazon Genomics CLI**
      @ `us-east-1`
      (because SRA s3 bucket is there)



Problems (1/2)

- **Current pipeline uses USEARCH, which is proprietary**
    - No FOSS!
    - Have license (>$1k), but *can only run 1 process at a time*, so no parallelization; so either run 6 years OR pay up to $1,000,000,000 for one million licenses :)
    - Alternative: use open source VSEARCH instead (but need refactoring)
- **Caching containers**
    - Some hundreds of Mb would need to be downloaded for each step if containers cannot be cached
    - Implement custom solution

Problems (1/2)

- **Staging persistent input files**
  - ~500 MB that would otherwise need to be downloaded for each step
  - Currently not possible based on specs (issue exists)
  - Need to come up with custom solution in ELIXIR::GA4GH Cloud until interoperable solution is agreed upon for TES
- **Staging inputs & outputs, managing intermediates**
  - Sample files (FASTQ) are not big (~100 MB), but >1,000,000 of them still means moving around and storing >100 TB!
  - Find out what's the most efficient way of transferring data (download in each process vs batch download vs download all of them)
  - Delete intermediates upon completion; possibly move out results (but "only" 4 TB for all runs)

Who pays the bill? :)

ELIXIR may cover, but not yet sure, working on it

Could use help of…

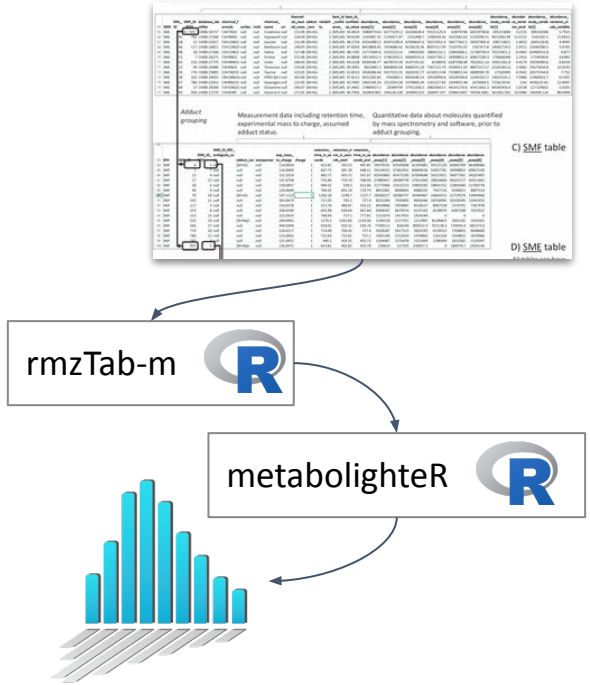
- Snakemake devs
- Anyone wishing to play with the ELIXIR::GA4GH Cloud :)

Improving interoperability support for authoring, editing and conversion of mzTab-M for Lipidomics Tools

Eduardo Jacobo Miranda Ackerman (MPI-CBG Dresden), Daniel Krause (FZ Borstel), Nils Hoffmann (FZ Jülich), Olena Mokshyna (IOCB Prague), w/ support by Steffen Neumann (IPB Halle)

mzTab-M Support - progress

- LipidXplorer writes mzTab-M (Jacobo)
- development of lxPostman support still ongoing (Daniel)
- R implementations
  - Google Colab Notebook for testing of conversion of mzTab-M to ISAtab for MetaboLights submission (using MTBL263 as an example) + mzMLs (Nils)
  - Writing of MAF file from mzTab-M (Steffen)
- MZmine 3 support (Olena)
  - testing of import function, documentation of current limits / issues
  - implementation and testing of export of mzTab-M
    - MZmine compound and spectral database annotations
- Help needed:
  - ISAtab creation (Study and assays from mzTab-M in R)
  - Configurable WebComponents for use in RShiny and Java Webapp for autocompletion of suitable CV terms (against existing REST API)
  - Anyone willing to participate in MZmine3 development (Java) is welcome



Towards a minimum information checklist for biomedical research projects with sensitive human data (only remote)

Pinar Alper, Vilém Děd, Christoph Kämpf, Valérie Barbié , Marina Popleteeva, Nene Djenaba Barry, Frédéric Erard

Recap

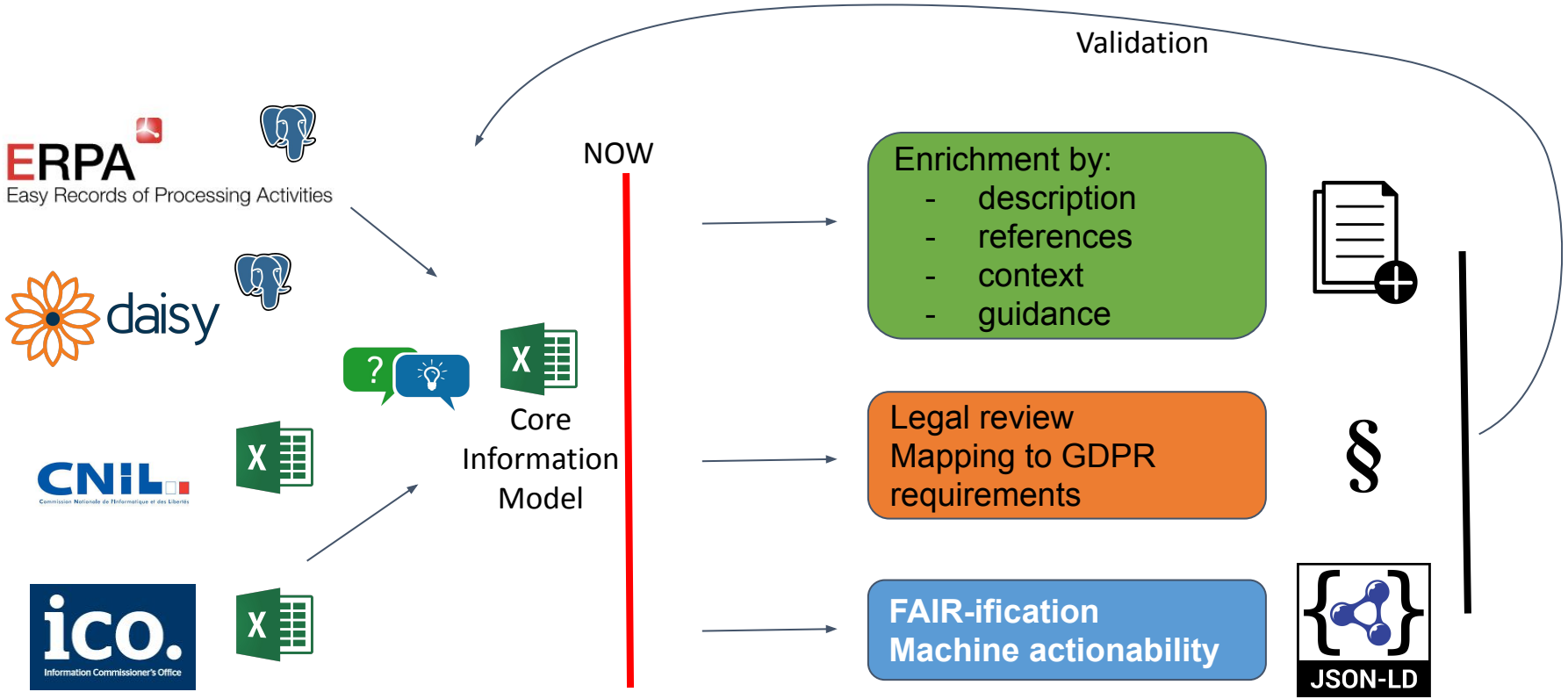
- The GDPR requires a written form for the Record of Processing Activities (Art. 30).
- The record **format can be chosen freely**, and it can be created on paper or numerically.
- Public organizations have to communicate the record to any person who demand it.

Reporting of sensitive data is big unknown for many stakeholders.

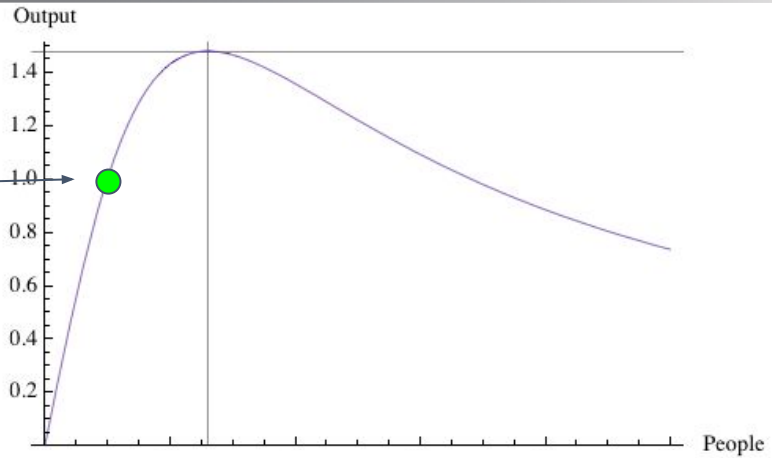
Lack of standards on format, content, scope, …

→ Minimal Information for Record Of Processing Activities (MIROPA)

Current progress / Next steps



We are here :)



Slack:
#checklist_for_human_data

Feel free to join if you have:

- Knowledge of minimal information checklists
- Machine actionable representations for checklists (JSON, JSON-LD)
- Interest in GDPR and legal requirements for processing of sensitive data
- Experience in sensitive data publishing
- Experience in reporting data processing to supervisory authorities