UNIVERSITÄT GREIFSWALD
Wissen lockt. Seit 1456

LARAsuite

full open source automation

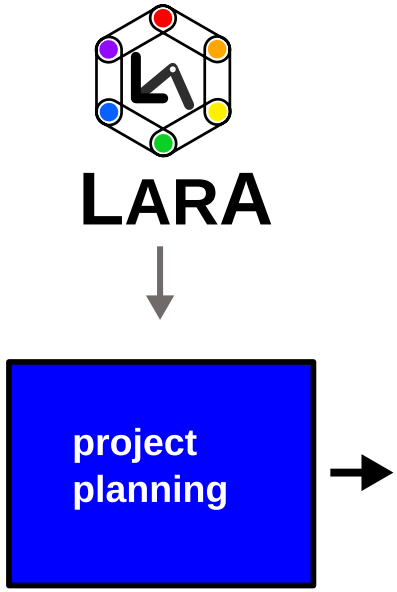
mark doerr, stefan maak & stefan born

university greifswald / tu-berlin

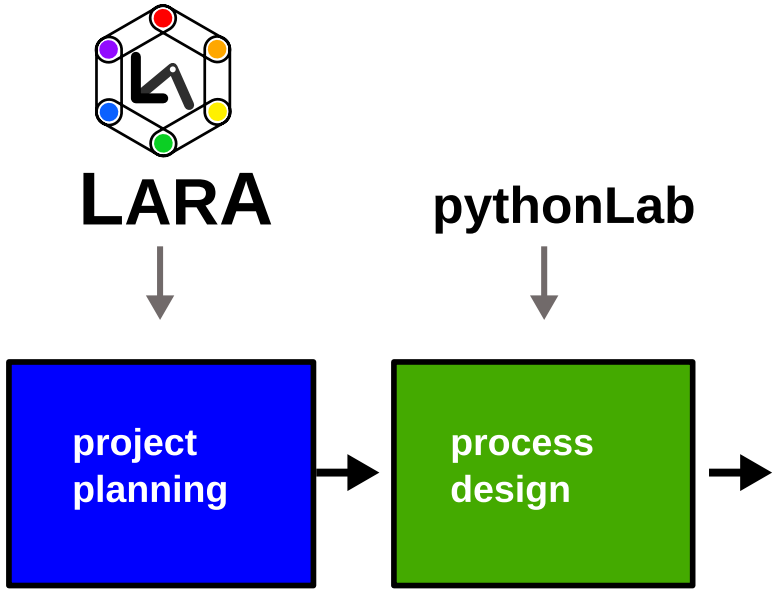
2024-10-11

LARA vision: a general purpose open source Lab Automation Infrastructure

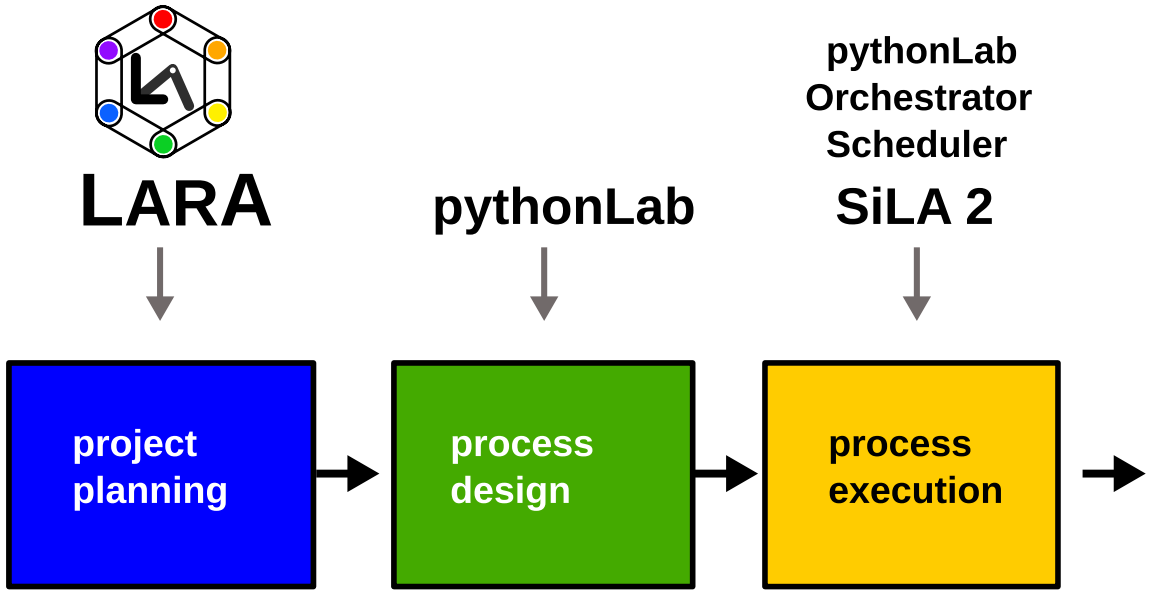
process planning



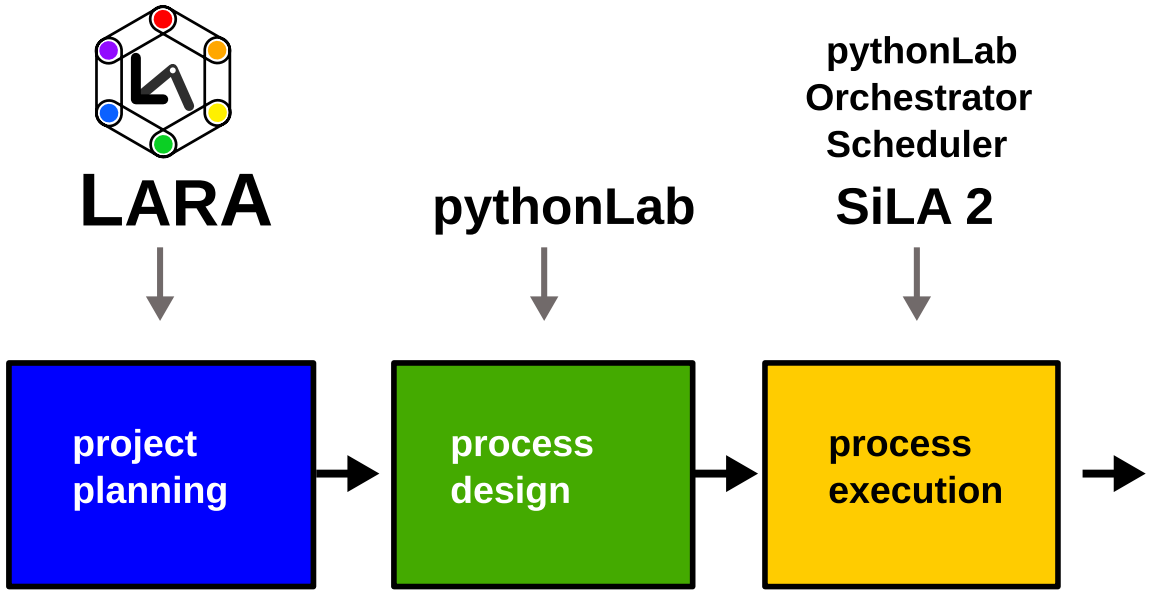
process design



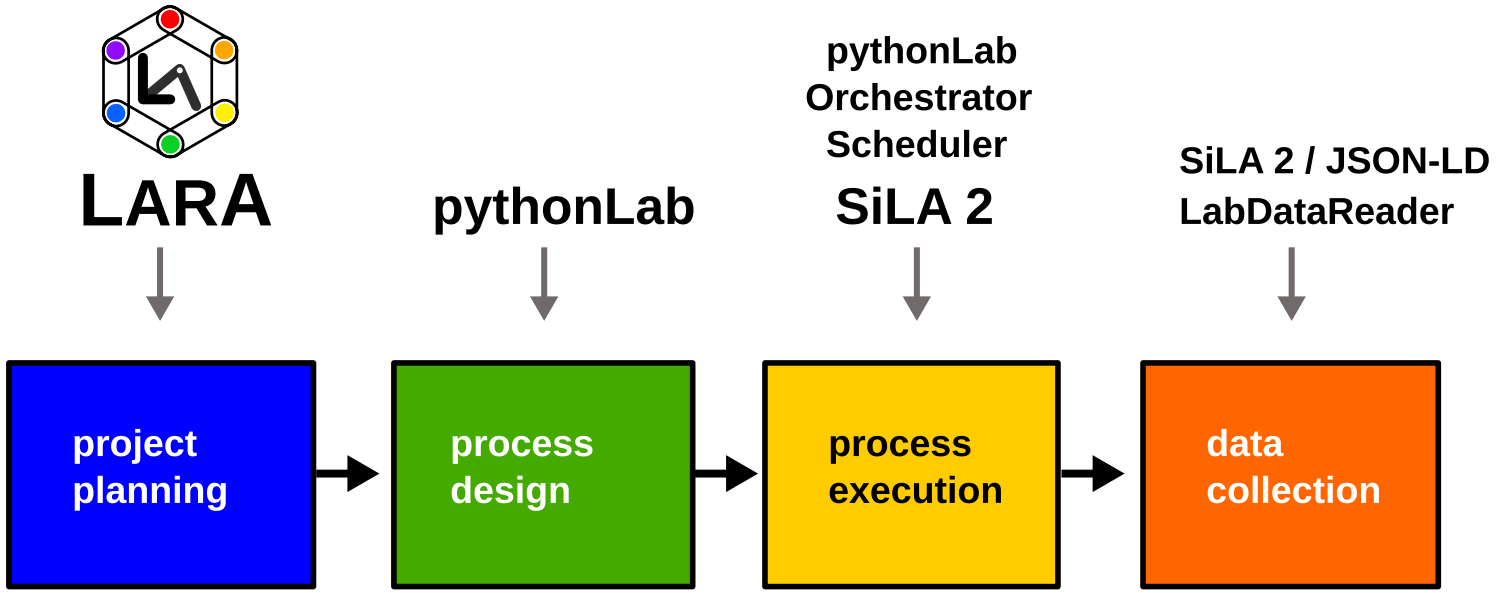
process execution



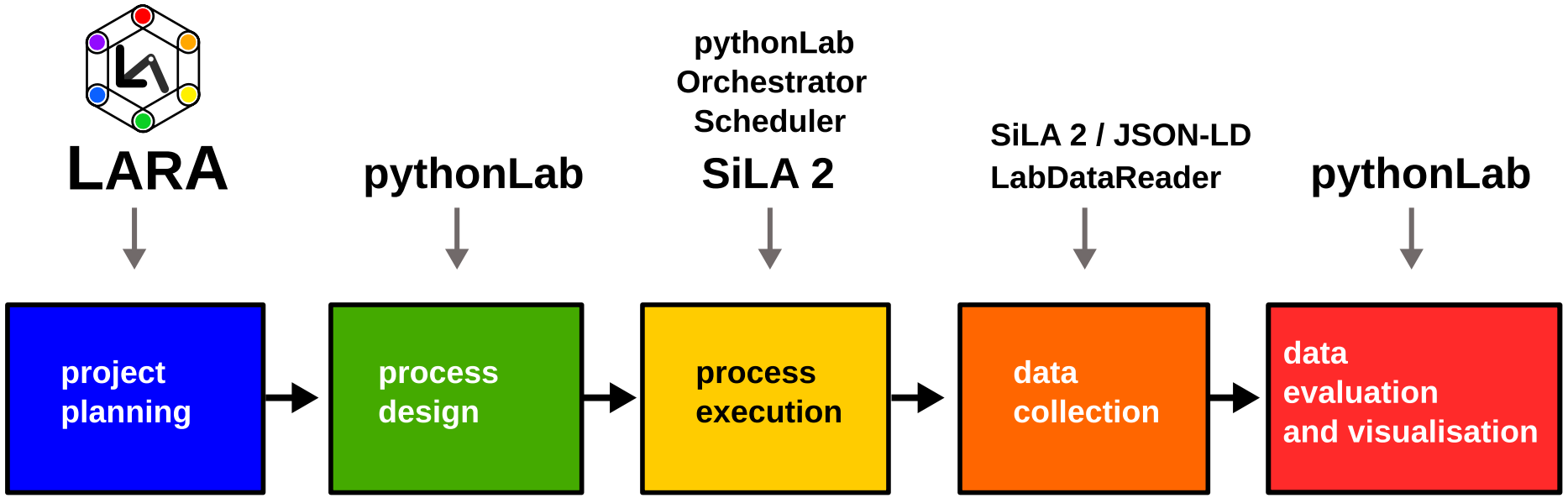
process execution



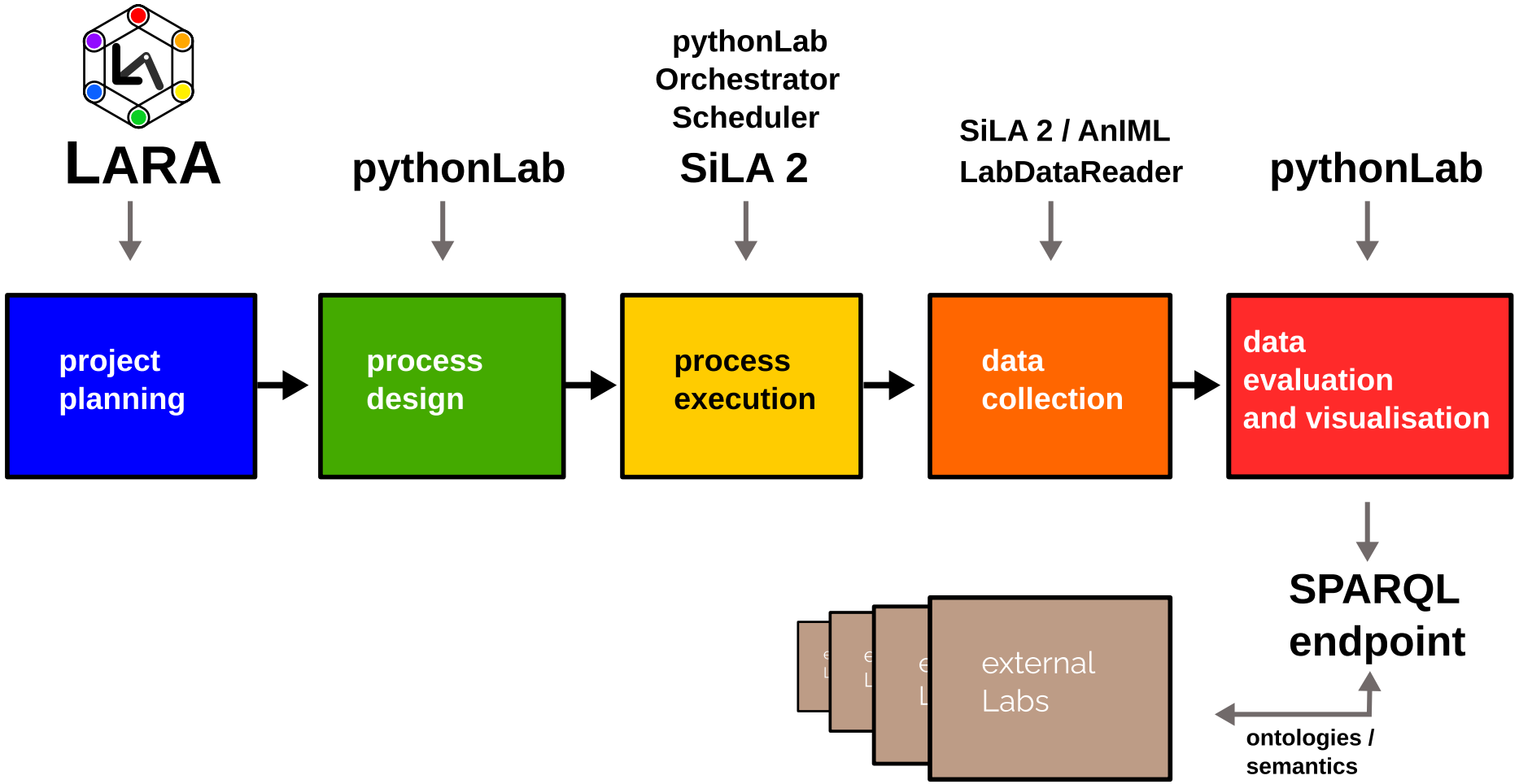
data collection



data evaluation / visualisation

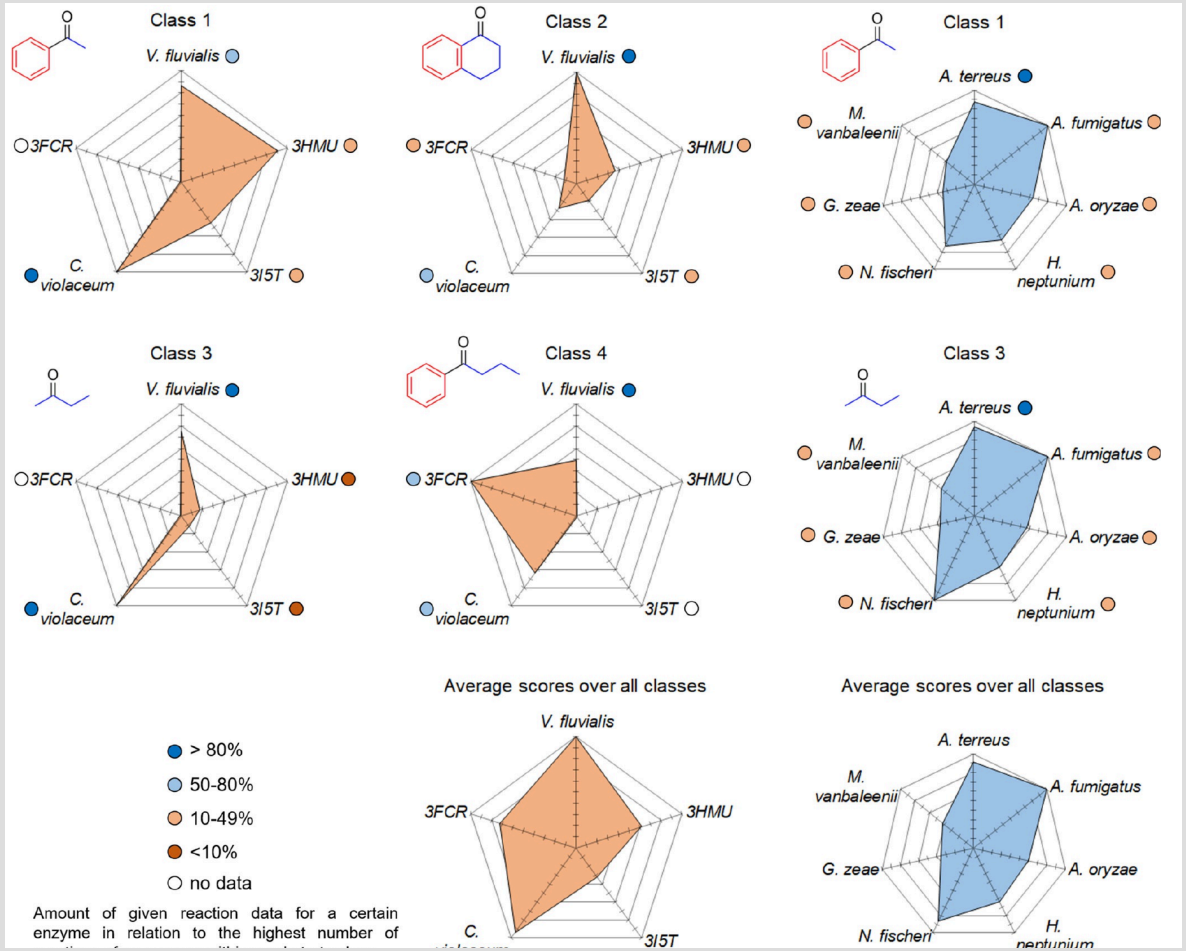


querying of data



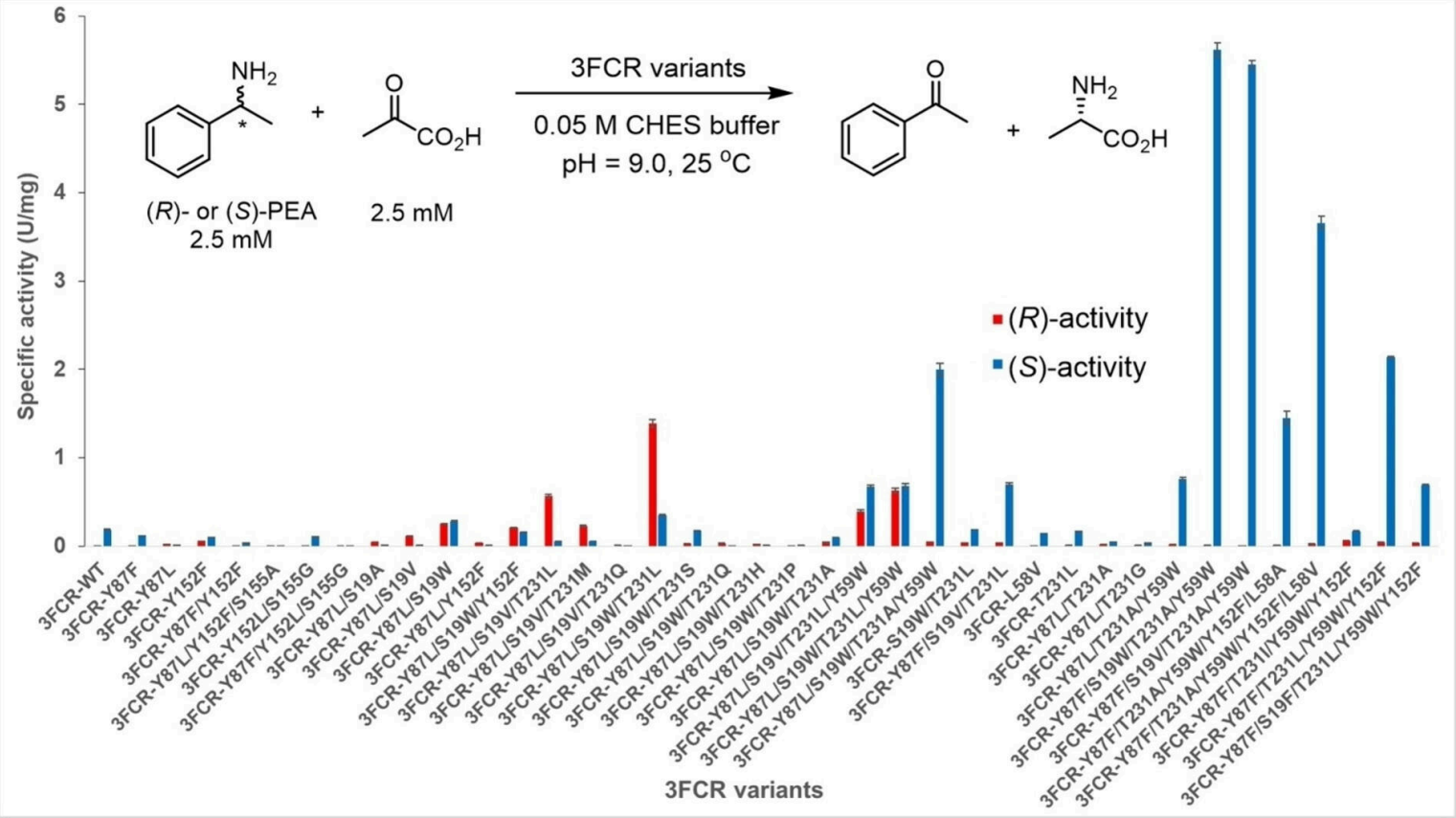
uni greifswald protein screening platform

protein engineering



Source: Calvelage, S. et al.; A Systematic Analysis of the Substrate Scope of (S)- and (R)-Selective Amine Transaminases. Advanced Synthesis & Catalysis 2017, 359 (23), 4235–4243. https://doi.org/10.1002/adsc.201701079.

machine learning



Source: Structure- and Data-Driven Protein Engineering of Transaminases for Improving Activity and Stereoselectivity Yu-Fei Ao et. al, Angewandte Chemie 2023. https://doi.org/10.1002/anie.202301660

motivation: why we need full automation of metadata aquisition and semantic data ?

semantic data

semantic data

- meaning of the data is well defined

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- machine readable

semantic data

- meaning of the data is well defined
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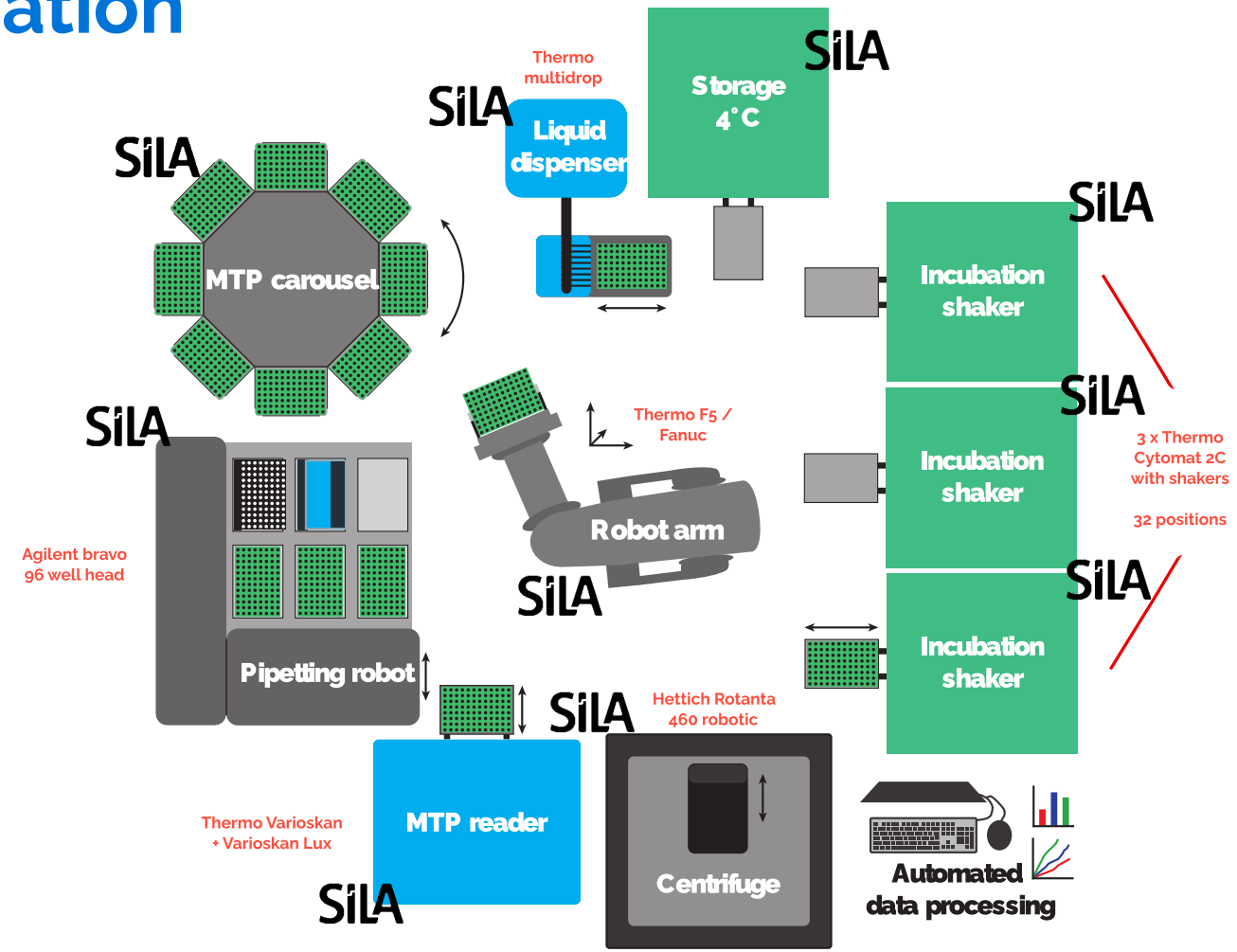
- machine actionable / “understandable”

semantic data

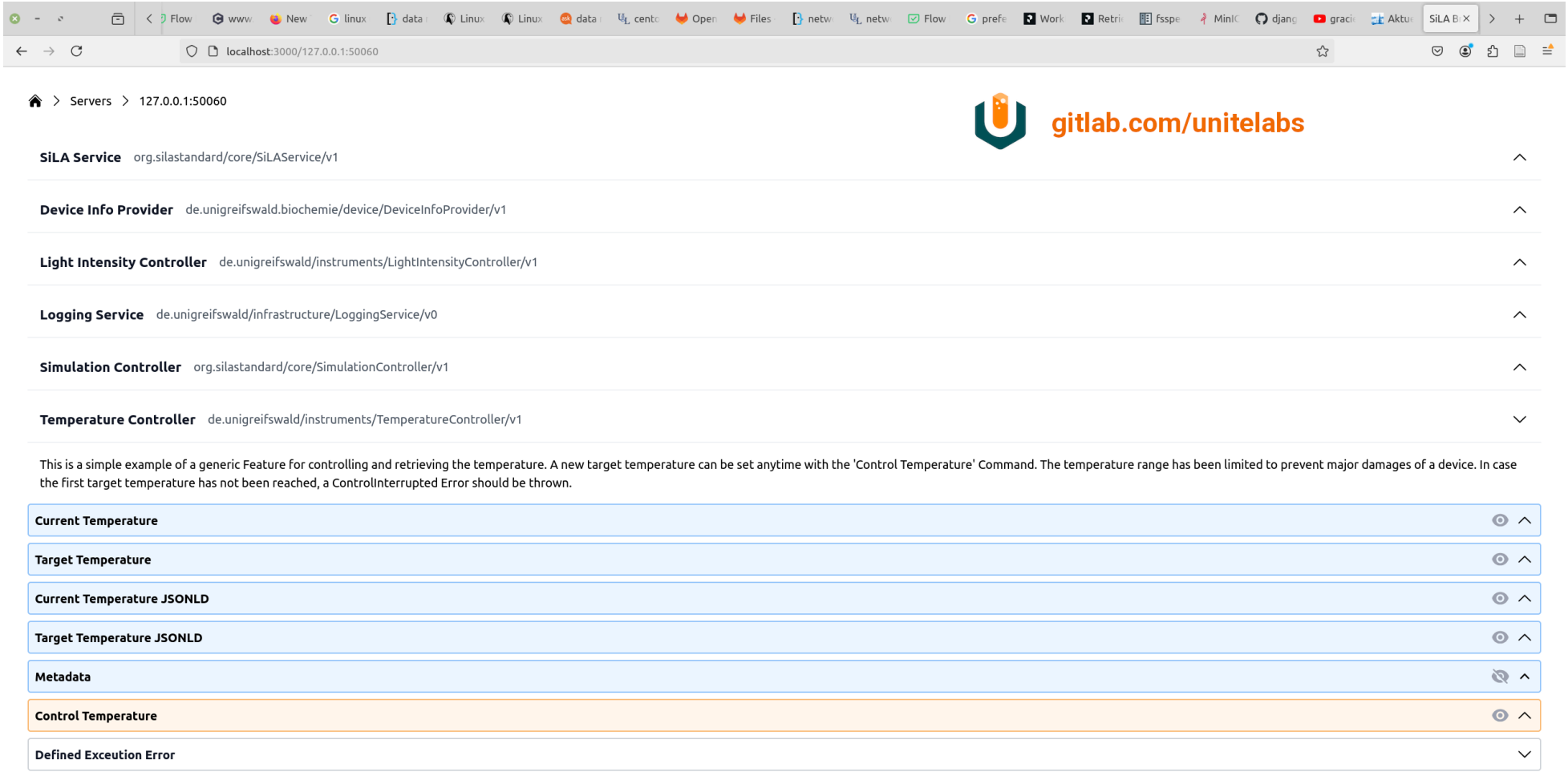
- meaning of the data is well defined
- machine readable
- machine actionable / “understandable”
- machine reasoning (inference) possible (reasoners)

https://en.wikipedia.org/wiki/FAIR_data

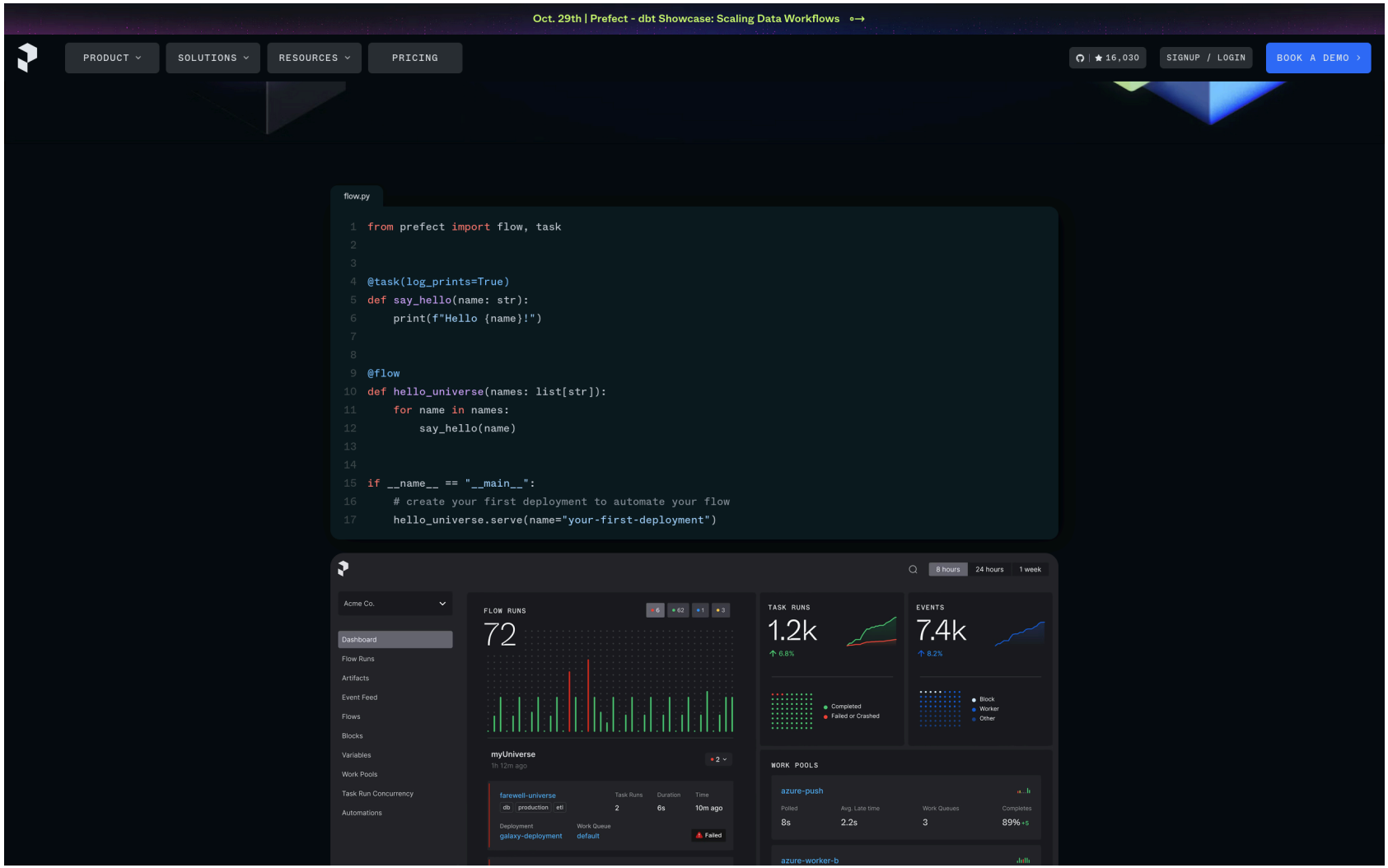
standardisation of communication



generic SiLA browser (unitelabs)



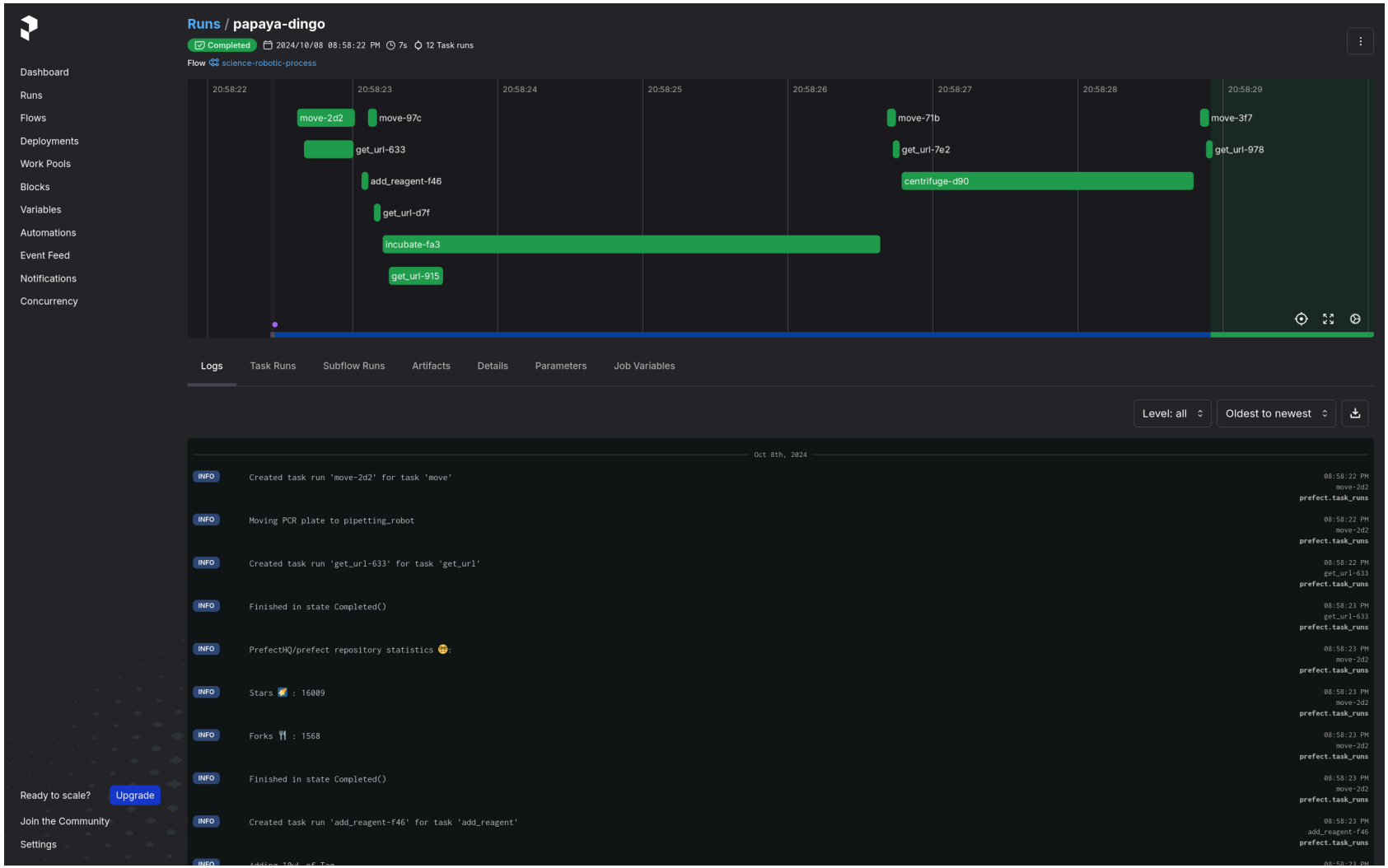
prefect (www.prefect.io)



demo : new LARAsuite orchestrator

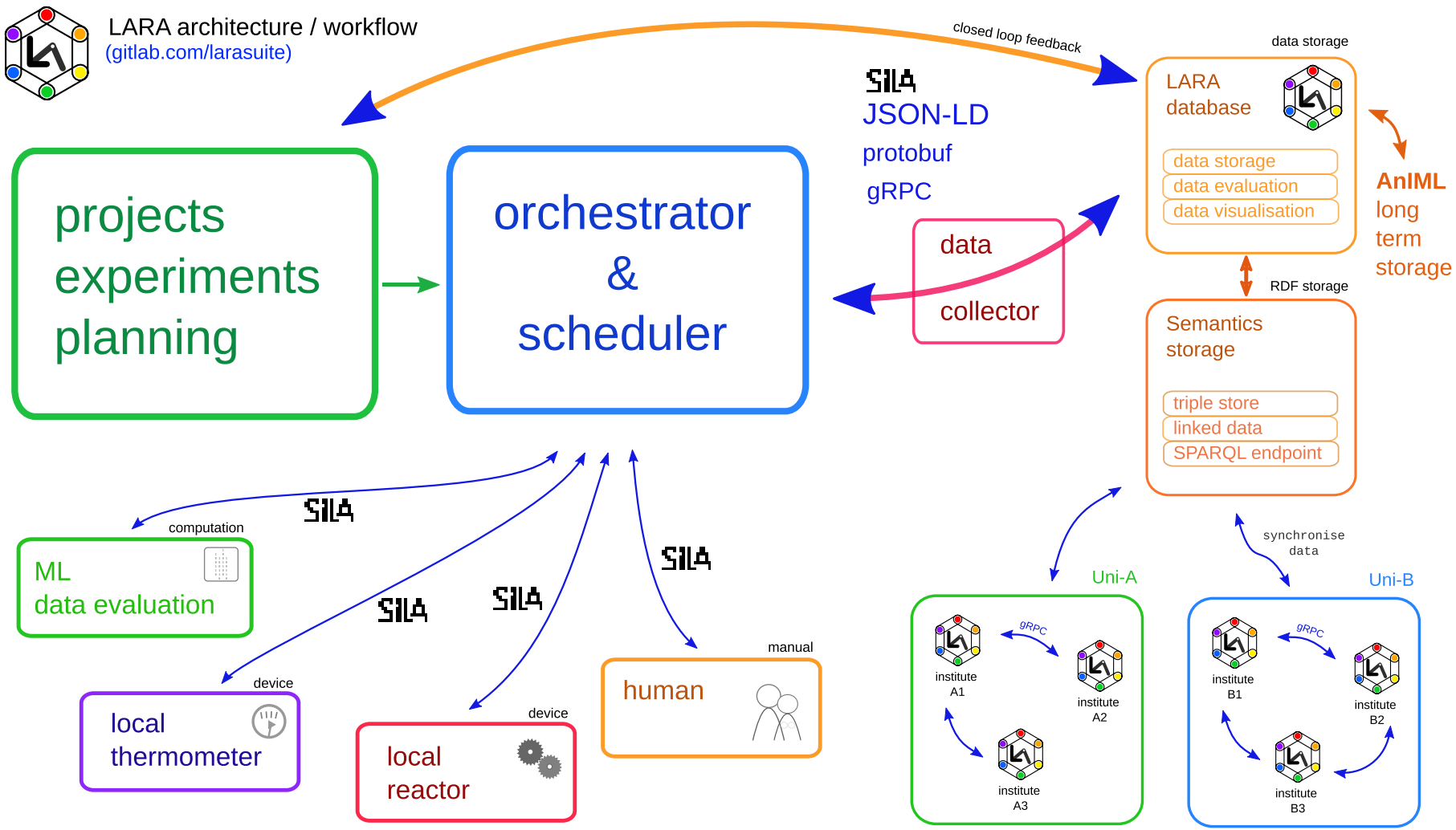
https://gitlab.com/larasuite

prefect 3 robotic workflow



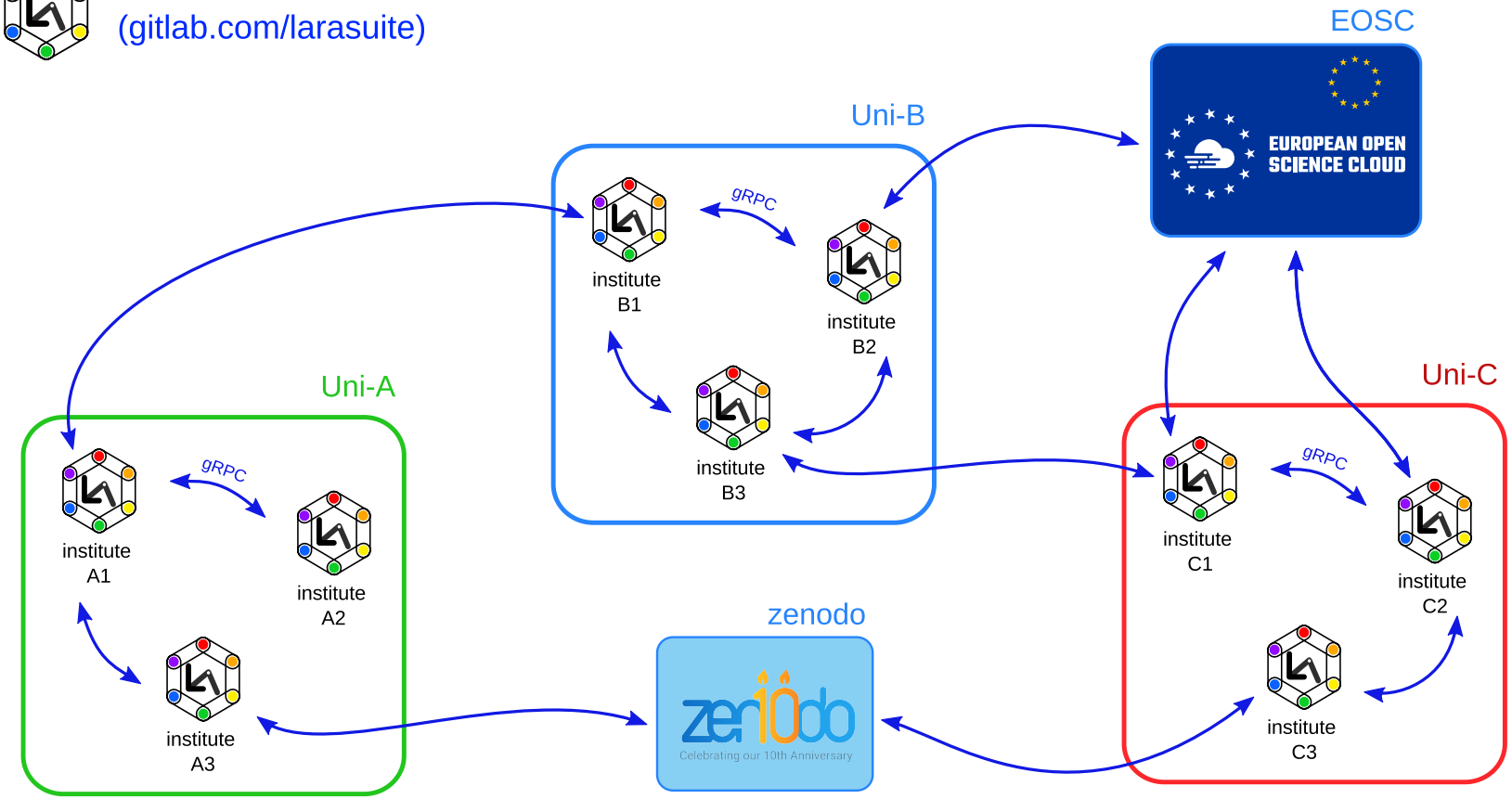
LARAsuite

LARAsuite overview



LARA connectivity

LARA network
(gitlab.com/larasuite)

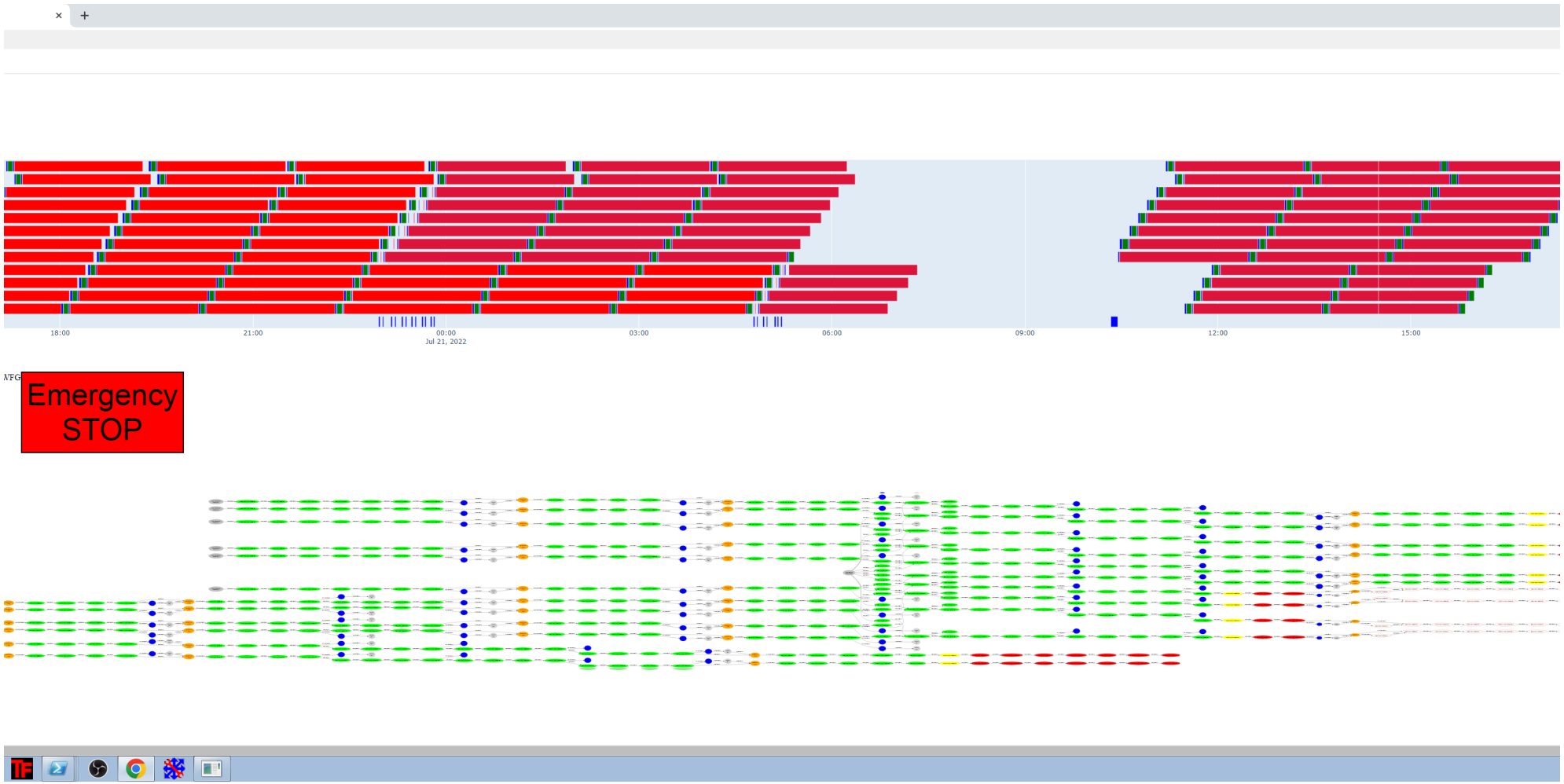


LARA pythonLab

```python
incubation_duration = 120
cont1 = self.containers[0]
# move to incubator
self.robot_arm.move(cont1, source_loc=cont1.pos, target_loc=self.incubator)
# incubate
self.incubator.incubate(cont1, duration=incubation_duration, temperature=310)
# move to reader
self.robot_arm.move(cont1, source_loc=cont1.pos, target_loc=self.reader)
# make absorbance measurement
self.reader.single_read(cont1, wavelengths=[600, 660], temperature=305)
# move back to hotel
self.robot_arm.move(cont1, source_loc=cont1.pos, target_loc=self.hotel)
```

https://gitlab.com/opensourcelab/pythonlab

LARA scheduler (Stefan Maak)



labDataReader

- generic reader of proprietary data (e.g. HPLC, plate readers)
- primary output : pandas data frame and *JSON-LD* (metadata)

https://gitlab.com/opensourcelab/scientificdata/labDataReader

SciDat

- packing tabular data / data frames into *parquet* files, including *JSON-LD* metadata

https://gitlab.com/opensourcelab/scientificdata/scidat

vocabulary and ontology developments

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- vocabularies - controlled vocabularies (example: github.com/nfdi4cat/voc4cat)

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- vocabularies - controlled vocabularies (example: github.com/nfdi4cat/voc4cat)
- taxonomies - hierarchical vocabularies
- ontologies - formal representation of knowledge with reasonig capabilities

vocabulary and ontology developments

https://forschungsdaten-thueringen.de/nfdi-en.html

and now for something completely different ....

GBA software / data workgroup

collection of atomic lab operations

- common workflow language ontology with a mapping infrastructure to translate this into execution workflows
- collection of competency questions for the ontology developments

https://gitlab.com/opensourcelab/scientificdata/ontologies/openscienceontology/experimental-workflows

semantically enriched data

- conversion of proprietory data to *JSON-LD* format

https://gitlab.com/opensourcelab/scientificdata/labdatareader

https://gitlab.com/opensourcelab/scientificdata/scidat

open source workflow orchestration environment

- for the members, who do not have software development skills

https://gitlab.com/opensourcelab

GBA software/data workgroup

- if you have more experiance, more ideas, better software development skills and infrastructures,

please support us ! (or take over ;)

acknowledgements

- Stefan Maak
- Uwe Bornscheuer's group (Univ. Greifswald)

project partners

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- Peter Neubauer's group (TU Berlin)
- Johannes Kabisch's group and associates (Uni Trondheim)
- Egon Heuson (Uni Lille)
- Lukas Bromig and Julian Willand (unitelabs)

KIWI-biolab team, NFDI4Cat teams, SiLA team & AnIML team

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lara.uni-greifswald.de/presentations