



LARA

the automation pipeline for BioCatalytic / Enzymatic
processes

mark doerr, stefan maak, stefan born & uwe bornscheuer

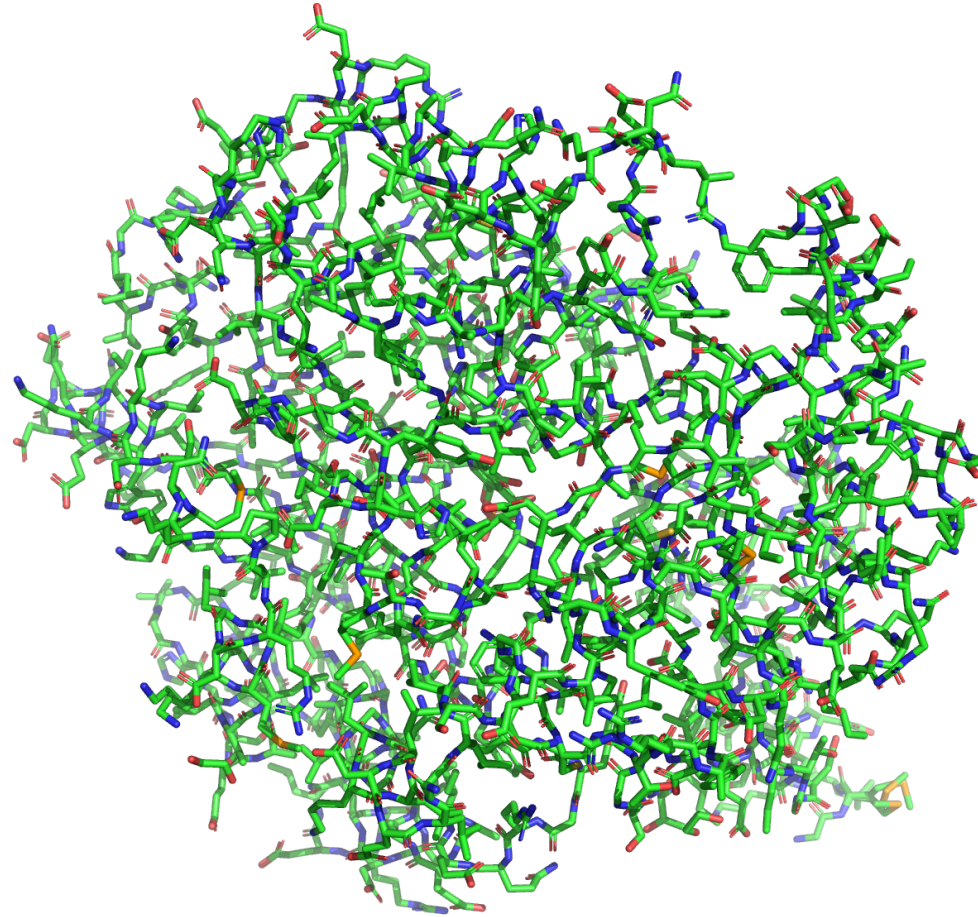
university greifswald / tu-berlin

2024-11-07

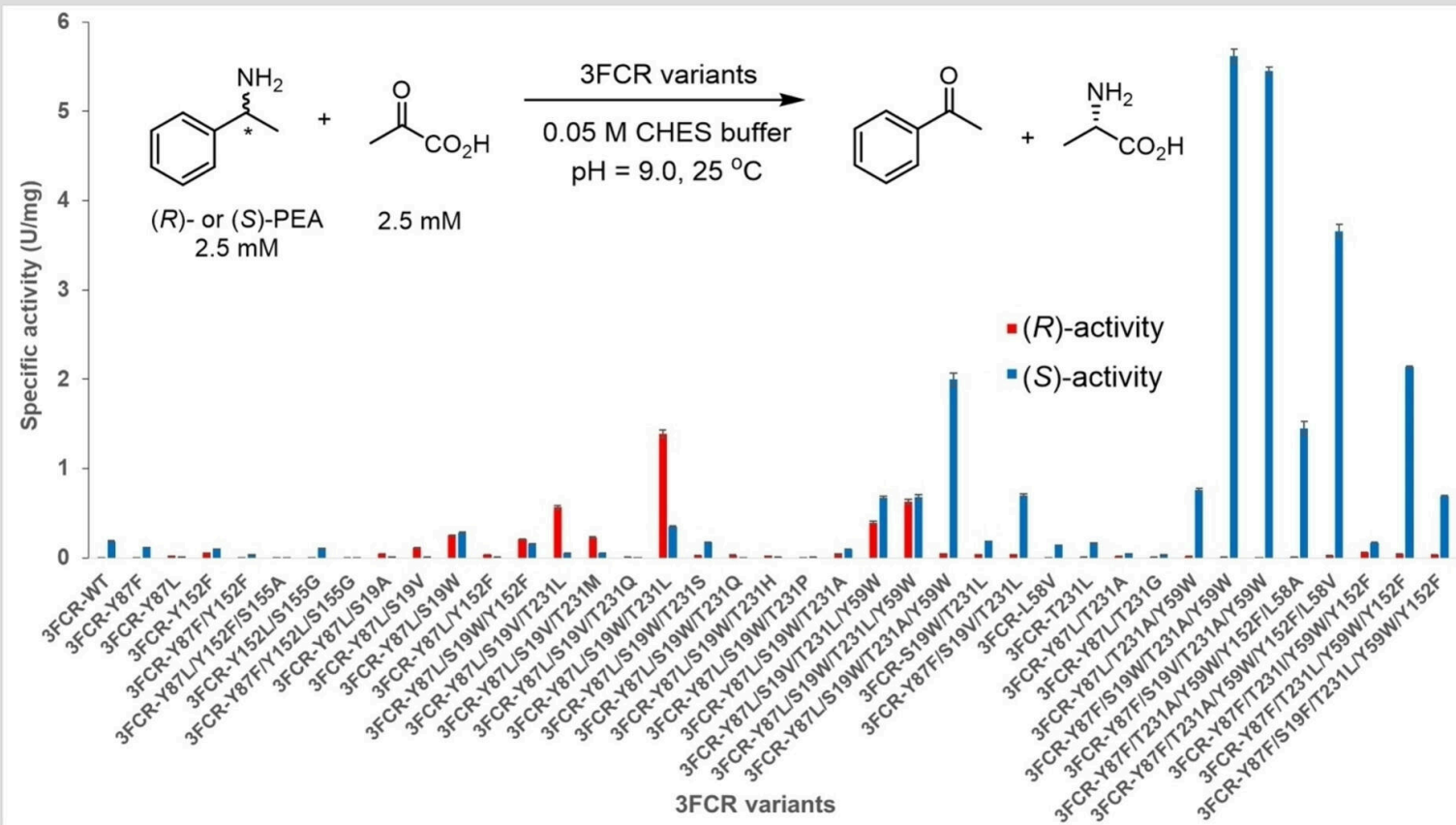
use case/motivation



machine learning

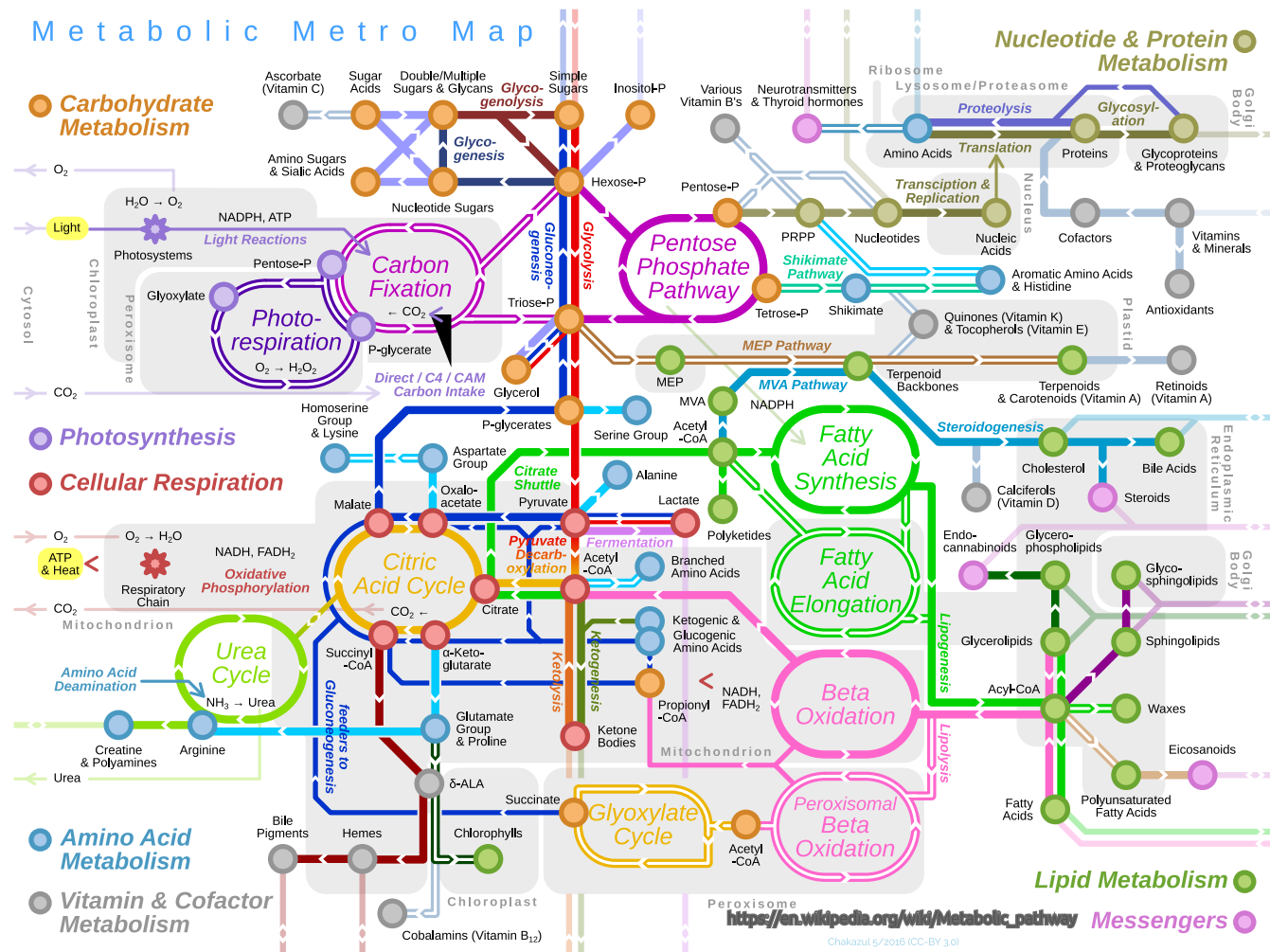


machine learning



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>

complex expression system



complex instrumentation



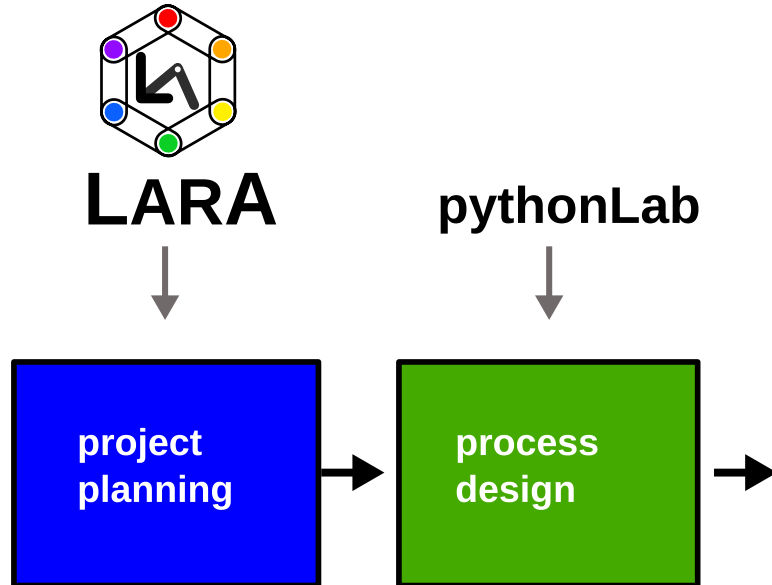


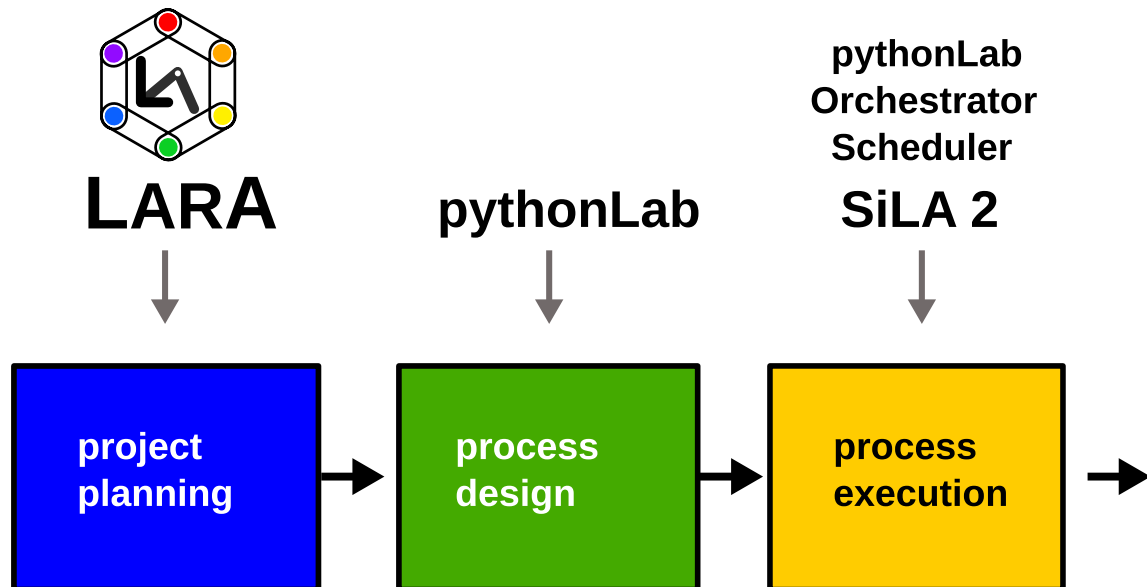
LARA

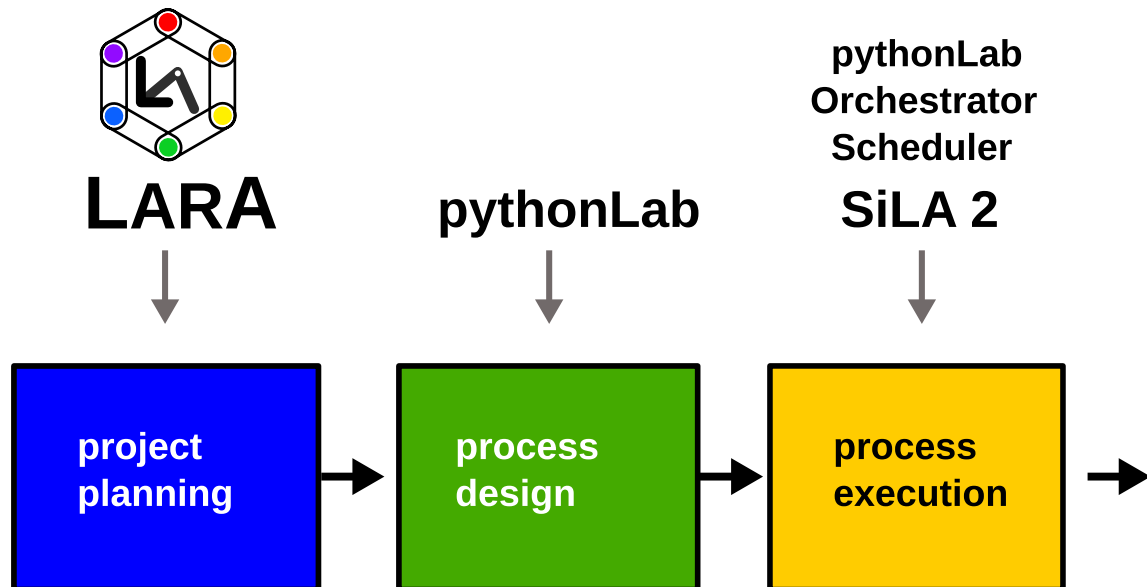


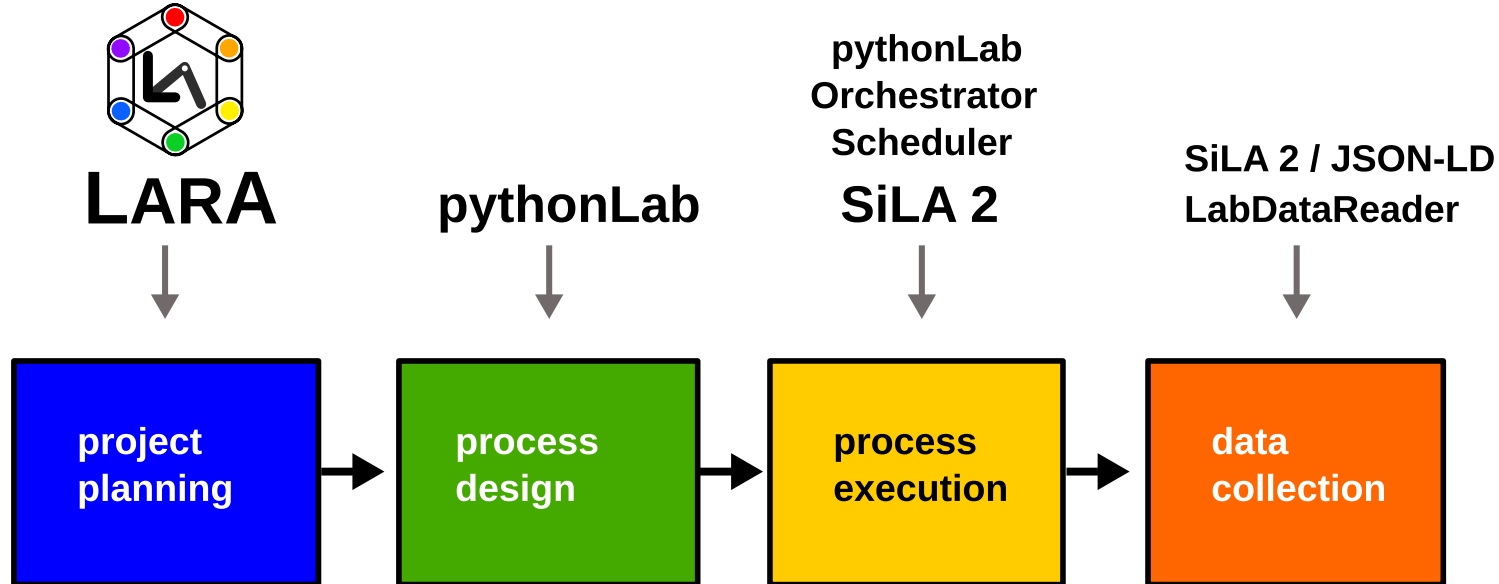
**project
planning**

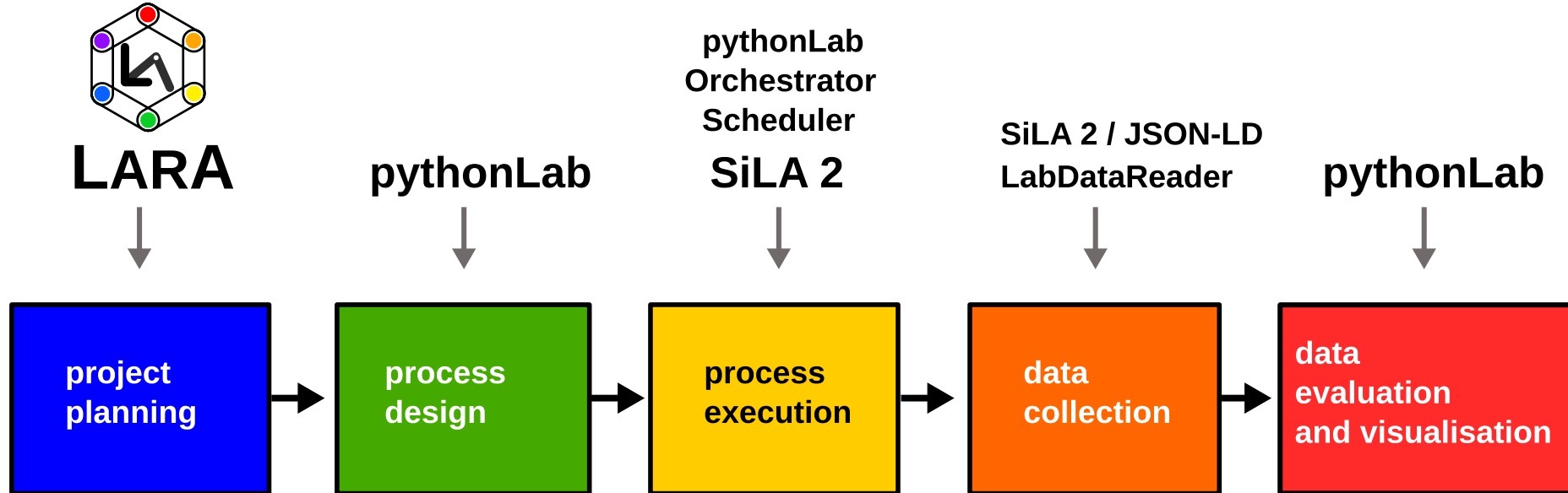


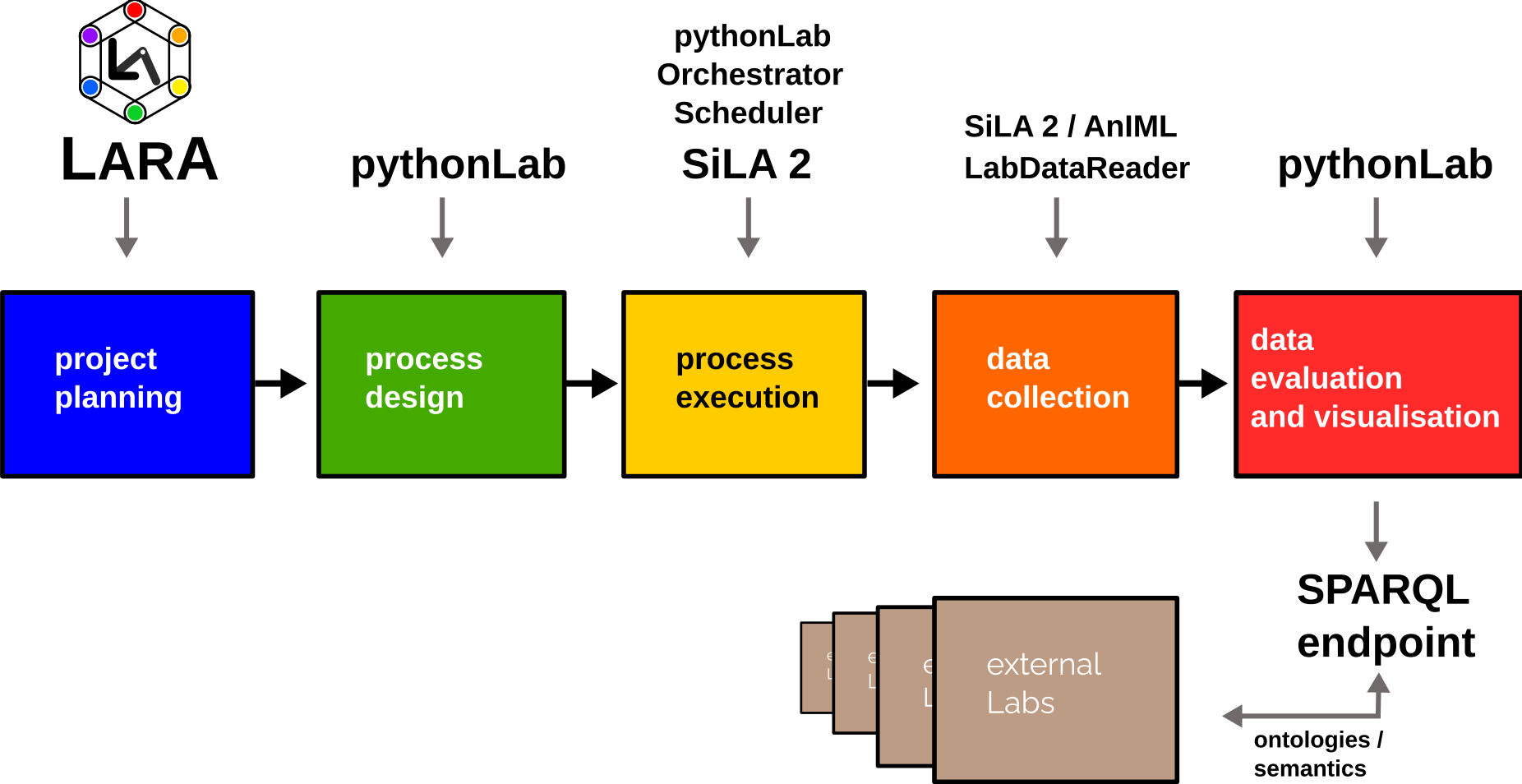


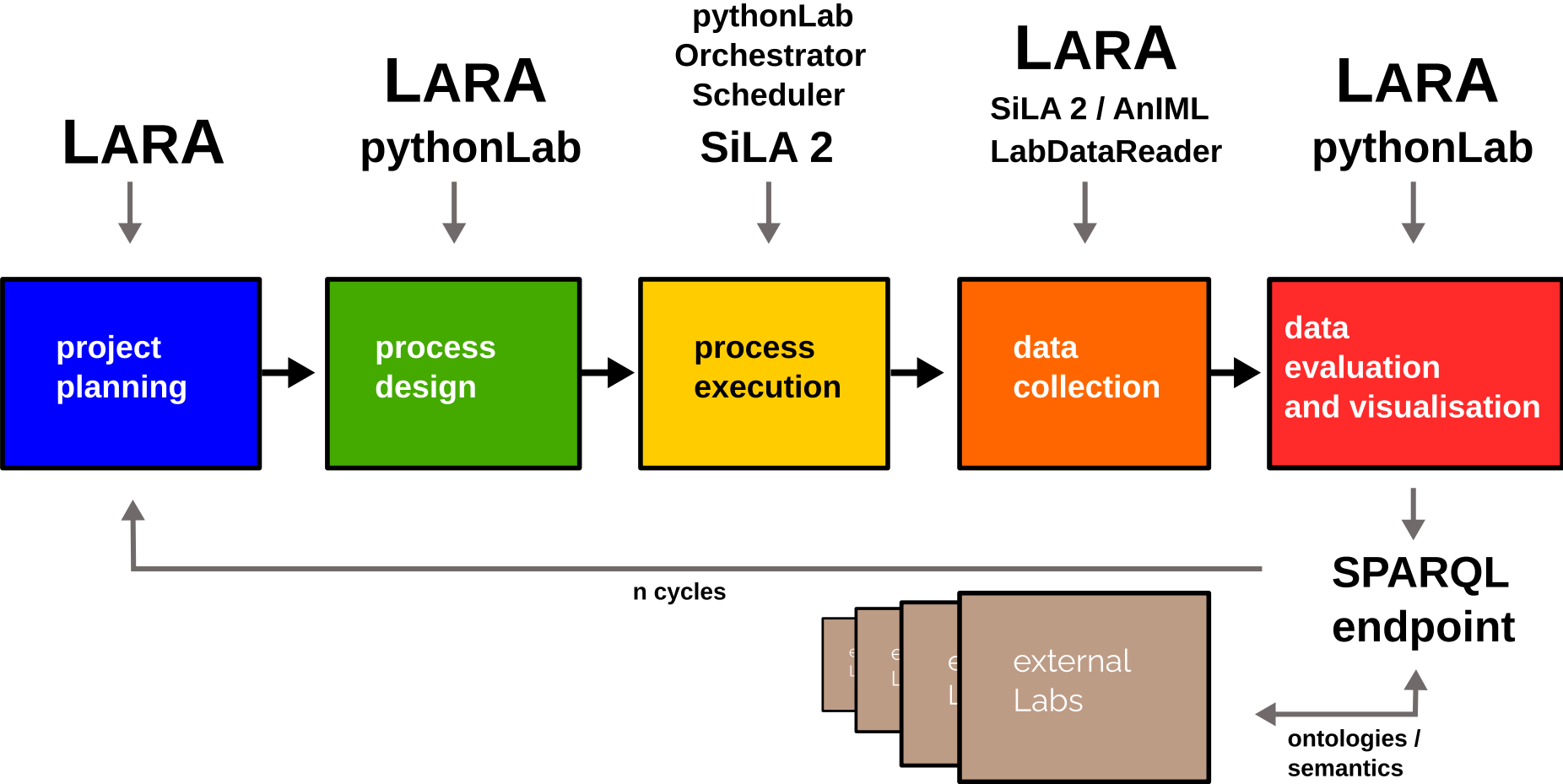












motivation: why we need full
automation of metadata
acquisition and semantic data ?

- meaning of the data is well defined

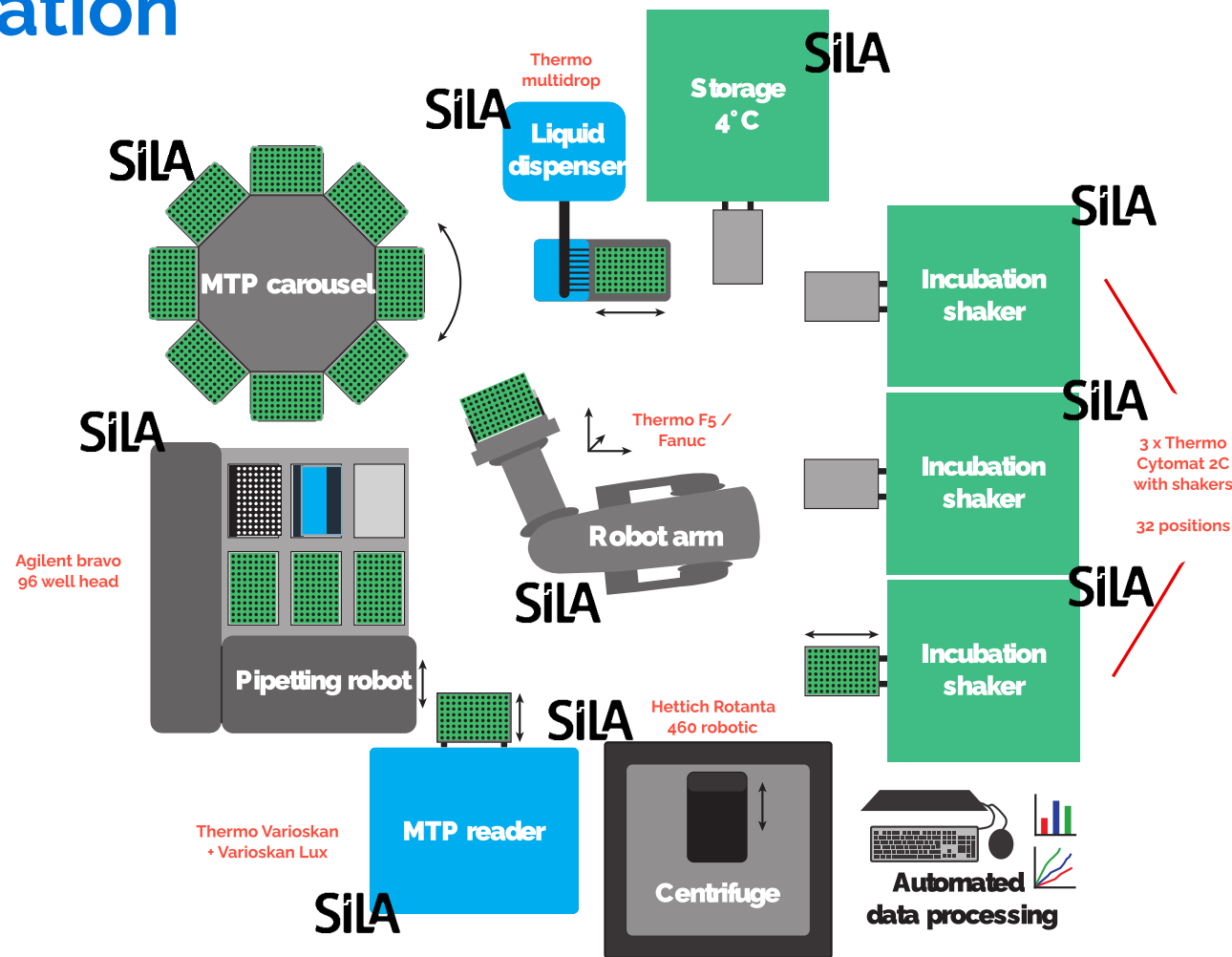
- meaning of the data is well defined
- machine readable

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

- 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



localhost:3000/127.0.0.1:50060

Servers > 127.0.0.1:50060

SiLA Service

org.silastandard/core/SiLAService/v1

^

Device Info Provider

de.unigreifswald.biochemie/device/DeviceInfoProvider/v1

^

Light Intensity Controller

de.unigreifswald/instruments/LightIntensityController/v1

^

Logging Service

de.unigreifswald/infrastructure/LoggingService/v0

^

Simulation Controller

org.silastandard/core/SimulationController/v1

^

Temperature Controller

de.unigreifswald/instruments/TemperatureController/v1

v

This is a simple example of a generic Feature for controlling and retrieving the temperature. A new target temperature can be set anytime with the 'Control Temperature' Command. The temperature range has been limited to prevent major damages of a device. In case the first target temperature has not been reached, a ControlInterrupted Error should be thrown.

Current Temperature

Target Temperature

Current Temperature JSONLD

Target Temperature JSONLD

Metadata

Control Temperature

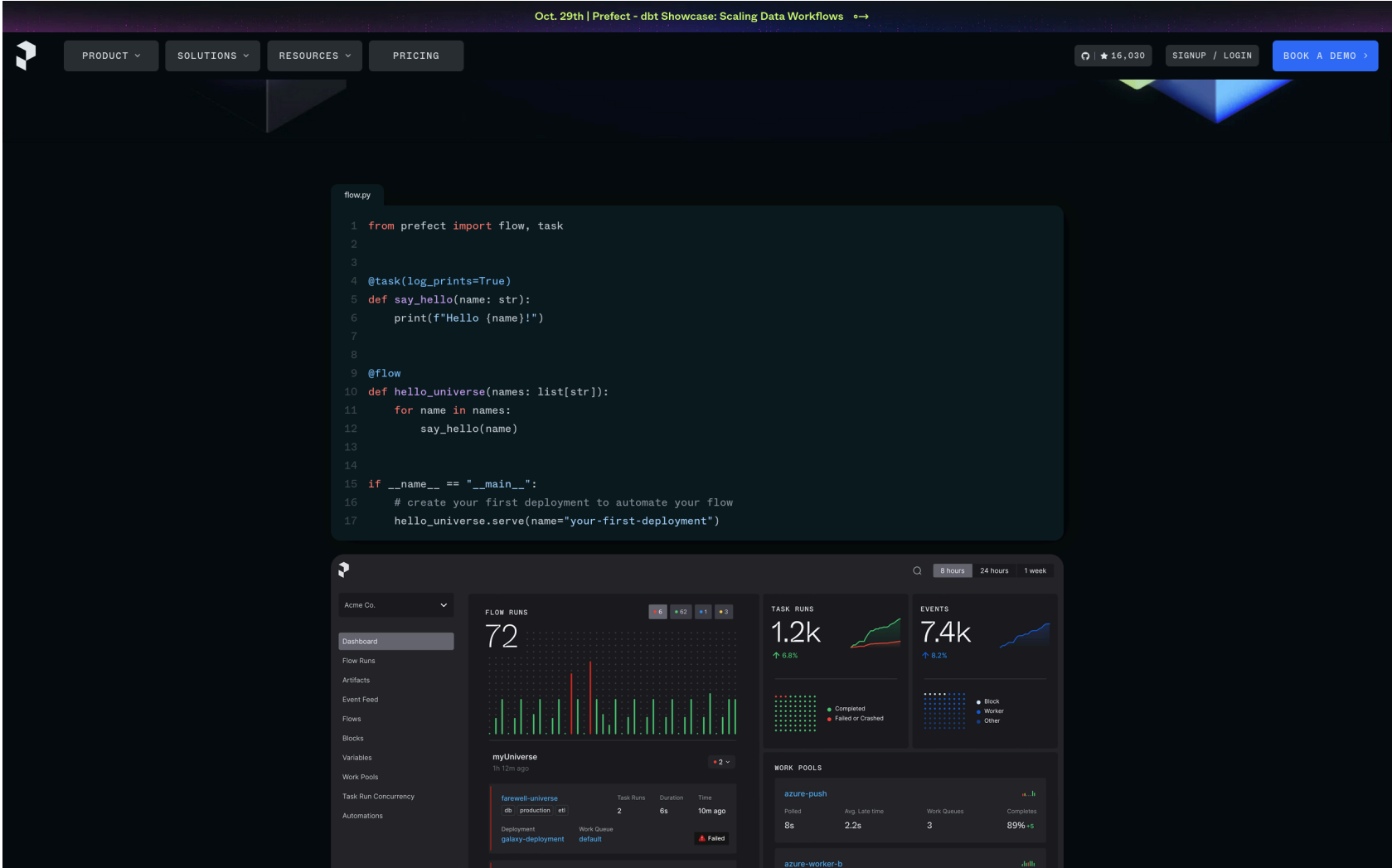
Defined Exceution Error

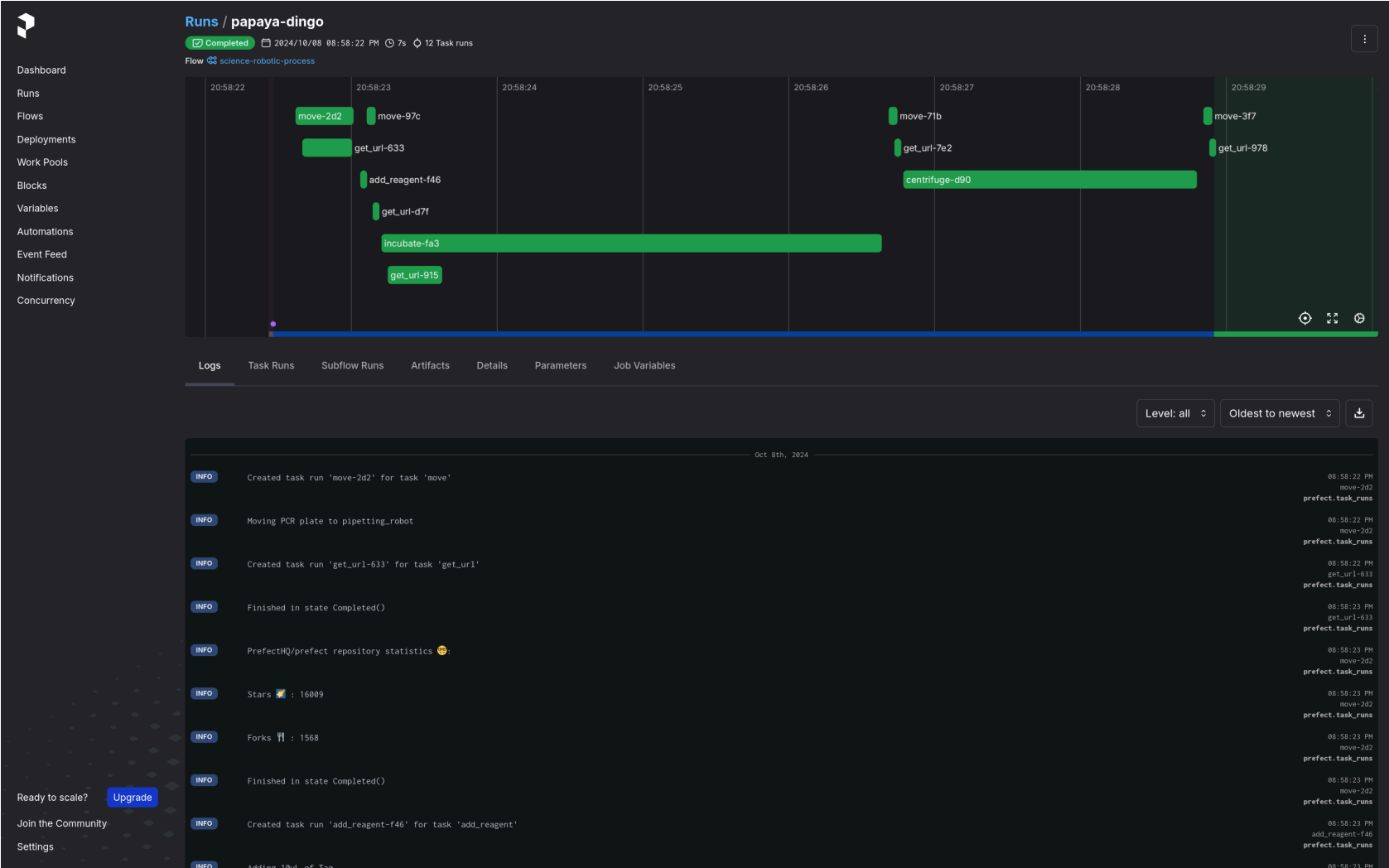
mark doerr

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LARAsuite

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[Admin](#)

LARA Main Modules - Apps

Projects

Management of Experiments and Projects.

[Projects](#)
[Experiments](#)

Processes

Management of Processes and Procedures.

[Procedures ...](#)
[Processes ...](#)
[Methods ...](#)

[Procedure Inst.](#)
[Process Inst.](#)
[Method Inst.](#)

People

People and Groups database.

[People...](#)

Data

Data database.

[Data](#)

Substances, Reactions, Structures

Substances, Polymers, Mixtures, Reactions and Structures databases.

[Substances ...](#)
[Polymers](#)
[Mixtures](#)
[Reactions](#)

[Substance Inst.](#)
[Polym.I.](#)
[Mixtures I.](#)
[React I.](#)

Sequences

Sequences database.

[Sequences ...](#)

Material, Parts, Devices and Labware

Material, Parts, Devices and Labware databases

[Parts](#)
[Devices](#)
[Labware](#)

[Parts I.](#)
[Devices I.](#)
[Labware I.](#)

Samples

Samples database .

[Samples ...](#)

Organisms

Organism databases

[Organisms ...](#)
[Organisms Inst.](#)

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LARA



SPARQL Query Editor

About

Tables

Conductor

Permalink

Extensions:

cxml

save to dav

sponge

User: SPARQL

Default Data Set Name (Graph IRI)

urn:spargl:lara:data

Query Text

```
SELECT *
WHERE {
    ?s ?p ?o .
}
LIMIT 30
```

Results Format

HTML

Execute Query

Reset

Execution timeout

0

milliseconds

Options

☒ Strict checking of void variables

☐ Log debug info at the end of output (has no effect on some queries and output formats)

☐ Generate SPARQL compilation report (instead of executing the query)

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Virtuoso version 07.20.3240 (a1fd8195b) on Linux (x86_64-ubuntu_focal-linux-gnu) Single Server Edition (47 GB total memory, 117 MB memory in use)

SPARQL | HTML5 table

s	p	o
http://w3id.org/lara/demo_data_1b_v0.0.1	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://www.w3.org/2002/07/owl#NamedIndividual
http://w3id.org/lara/demo_data_1c_v0.0.1	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://www.w3.org/2002/07/owl#NamedIndividual
http://w3id.org/lara/demo_data_1b_v0.0.1	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://w3id.org/lara/Data
http://w3id.org/lara/demo_data_1c_v0.0.1	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://w3id.org/lara/Data
http://w3id.org/lara/demo_data_1b_v0.0.1	http://w3id.org/lara/datetime_last_modified	2024-11-06T08:24:08.575Z
http://w3id.org/lara/demo_data_1c_v0.0.1	http://w3id.org/lara/datetime_last_modified	2024-11-06T08:24:17.634Z
http://w3id.org/lara/demo_data_1b_v0.0.1	http://w3id.org/lara/version	"v0.0.1"^^<http://www.w3.org/2001/XMLSchema#string>
http://w3id.org/lara/demo_data_1c_v0.0.1	http://w3id.org/lara/version	"v0.0.1"^^<http://www.w3.org/2001/XMLSchema#string>
http://w3id.org/lara/demo_data_1b_v0.0.1	http://w3id.org/lara/datetime_created	2024-11-06T09:24:07.308Z
http://w3id.org/lara/demo_data_1c_v0.0.1	http://w3id.org/lara/datetime_created	2024-11-06T09:24:15.938Z
http://w3id.org/lara/demo_data_1b_v0.0.1	http://w3id.org/lara/name_full	"https://de.unigreifswald/biochem/akb/demo_data_1b_v0.0.1"^^<http://www.w3.org/2001/XMLSchema#string>
http://w3id.org/lara/demo_data_1c_v0.0.1	http://w3id.org/lara/name_full	"https://de.unigreifswald/biochem/akb/demo_data_1c_v0.0.1"^^<http://www.w3.org/2001/XMLSchema#string>
http://w3id.org/lara/demo_data_1b_v0.0.1	http://w3id.org/lara/data_id	"48e9088d-9476-4f0e-90f8-c7923939266e"^^<http://www.w3.org/2001/XMLSchema#string>
http://w3id.org/lara/demo_data_1c_v0.0.1	http://w3id.org/lara/data_id	"627d3639-f41a-428b-87a0-a208fa8150a2"^^<http://www.w3.org/2001/XMLSchema#string>
http://w3id.org/lara/demo_data_1b_v0.0.1	http://w3id.org/lara/title	"Demo Data 1b"^^<http://www.w3.org/2001/XMLSchema#string>
http://w3id.org/lara/demo_data_1c_v0.0.1	http://w3id.org/lara/title	"Demo Data 1c"^^<http://www.w3.org/2001/XMLSchema#string>

SPARQL Query Editor

AboutTables

ConductorPermalink

Extensions: cxmlsave to davspongeUser: SPARQL

Default Data Set Name (Graph IRI)

urn:spargl:lara:data

Query Text

```
PREFIX rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX emmo: <http://emmo.info/emmo-inferred#>
PREFIX xsd: <http://www.w3.org/2001/XMLSchema#>
PREFIX lara: <http://w3id.org/lara/>

SELECT ?data_title ?date ?data_id
WHERE
{
  ?data lara:datetime_created ?date .
  ?data lara:data_id ?data_id .
  ?data lara:title ?data_title .
  FILTER (?date > "2024-11-01T00:00:00Z"^^xsd:dateTime)
}
LIMIT 30
```

Results Format

HTML

Execute Query

Reset

Execution timeout

0

milliseconds

Options

☒ Strict checking of void variables

☐ Log debug info at the end of output (has no effect on some queries and output formats)

☐ Generate SPARQL compilation report (instead of executing the query)

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[Virtuoso](#) version 07.20.3240 (a1fd8195b) on Linux (x86_64-ubuntu_focal-linux-gnu) Single Server Edition (47 GB total memory, 117 MB memory in use)

SPARQL | HTML5 table

data_title	date	data_id
"Demo Data 1b"^^<http://www.w3.org/2001/XMLSchema#string>	2024-11-06T09:24:07.308Z	"48e9088d-9476-4f0e-90f8-c7923939266e"^^<http://www.w3.org/2001/XMLSchema#string>
"Demo Data 1c"^^<http://www.w3.org/2001/XMLSchema#string>	2024-11-06T09:24:15.938Z	"627d3639-f41a-428b-87a0-a208fa8150a2"^^<http://www.w3.org/2001/XMLSchema#string>

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>

LARA is a tool ...

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- for planning, executing and evaluating experiments as complex as BioCatalytic / Enzymatic processes

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- leverages automation in many steps

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- leverages automation in many steps
- generates a knowledge graph on the fly

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- for planning, executing and evaluating experiments as complex as BioCatalytic / Enzymatic processes
- leverages automation in many steps
- generates a knowledge graph on the fly
- synchronises with external data sources (like Dataverse)

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- Egon Heuson (Uni Lille)
- Lukas Bromig and Julian Willand (unitelabs)

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