

A large, dark blue circular graphic on the left side of the slide. It features a central dark blue circle surrounded by a ring of lighter blue segments, resembling a stylized atom or a molecular structure. The background of the slide is a dark blue gradient with large, overlapping circular shapes.

Combining high-performance computing, workflows and ML to get new insights in material sciences

NHR4CES Community Workshop 2025 – Michael Selzer, Giovanna Tosato

1. Introduction

2. Kadi4Mat

3. KadiAI and CIDS

- Active Learning Optimization Framework

4. Tools and usecases:

- Model Parametrization for Solid Oxide Fuel Cells
- Outlook: Human-in-the-loop, automatized experiments

5. Conclusion

Introduction

1

Motivation

- Research data play an increasingly important role in almost all research disciplines, but their structured management is often neglected
 - **Research community:** Lack of reproducibility of research results, no data exchange, data loss (→ duplication of work)
 - **Data science:** Not only require large amounts of data, but the data must be of high quality and machine operable

→ Funding institutions also require a **FAIR research data management**



Deutsche
Forschungsgemeinschaft

<https://www.dfg.de>



Bundesministerium
für Bildung
und Forschung

<https://www.bmbf.de>

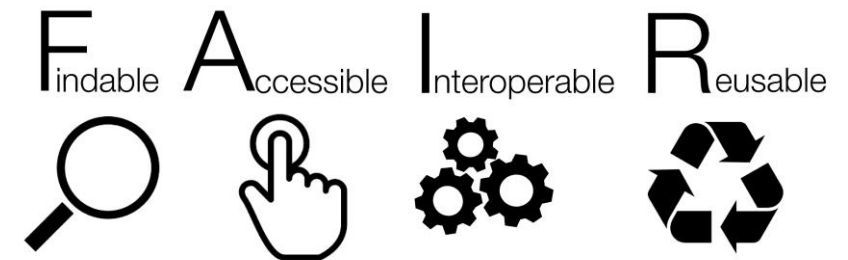
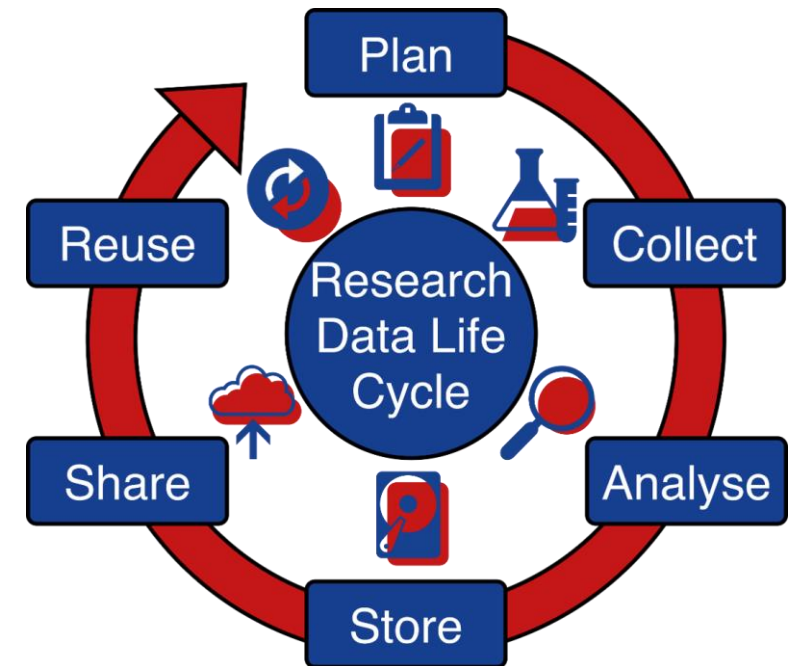


European
Commission

<https://commission.europa.eu>

Research Data Management (RDM)

- A structured RDM requires flexible solutions in order to accommodate user- and discipline-specific applications
- **Goals**
 - Consideration of all phases of the research data life cycle, where possible
 - Support of "step-by-step" FAIRness of data at different levels
 - Generic functionalities and integration of existing standards and systems → complementing instead of replacing



https://de.wikipedia.org/wiki/FAIR-Prinzipien#/media/Datei:FAIR_data_principles.jpg

Kadi4Mat

2

Kadi4Mat

- Kadi4Mat is the open source **research data infrastructure** that is being actively developed in the context of various research projects
- Originally developed in the context of materials science, it can be used for the management of any type of research data or process within any research discipline
- Multiple instances of Kadi4Mat are hosted at KIT [1] and other institutes, including a publicly available instance at <https://demo-kadi4mat.iam.kit.edu/>*



Kadi⁴Mat

Karlsruhe Data Infrastructure
for Materials Science

[1] <https://kadi.iam.kit.edu/#instances>

Conceptual Overview of Kadi4Mat

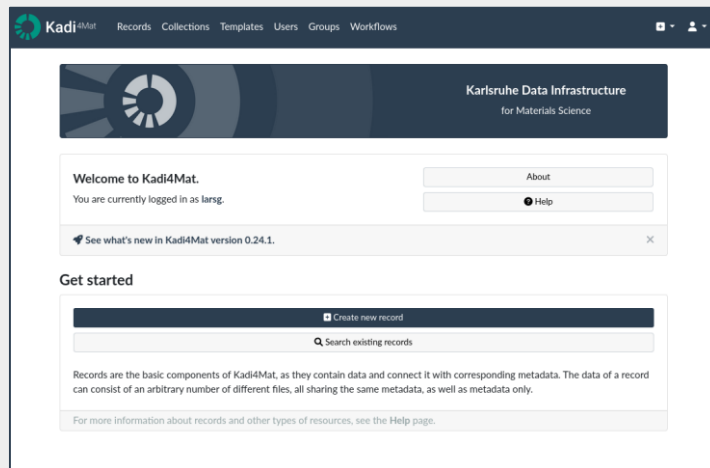
- The concept of **Kadi4Mat** is a modular and generic architecture that combines and interfaces with functionalities of **ELNs** and **repositories**



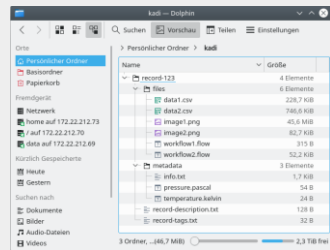
- The ELN part can be described as **ELN 2.0**, with focus on automation via a web-based API and data provenance (data origin), besides typical ELN functionality
- The repository part can be described as **community repository**, with focus on managing and sharing *warm data* (data yet to be analysed/processed further) within a community

The Kadi Ecosystem

KadiWeb Repository / Web



KadiFS Filesystem

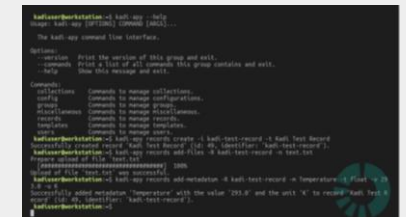


Streamline
your
research

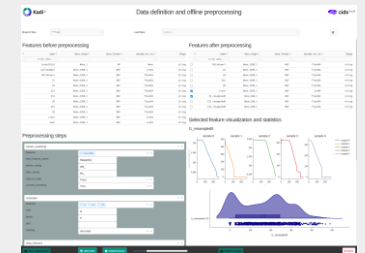
KadiStudio Workflows



KadiAPY (Python) API

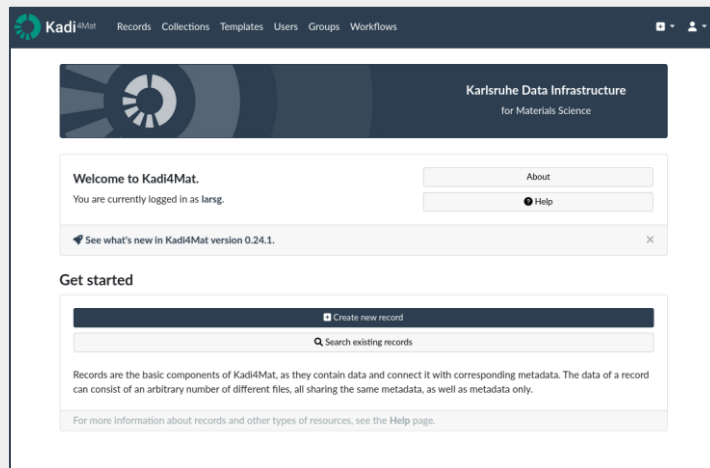


KadiAI ML Interface

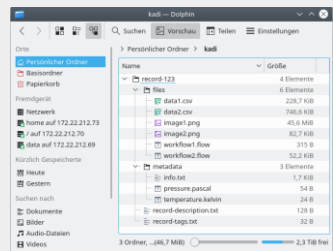


The Kadi Ecosystem

KadiWeb Repository / Web



KadiFS Filesystem

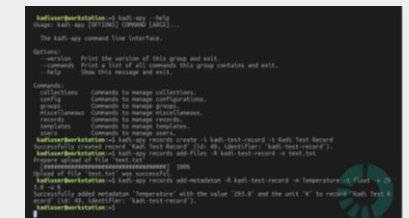


Streamline
your
research

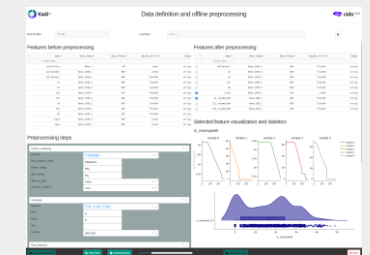
KadiStudio Workflows



KadiAPY (Python) API



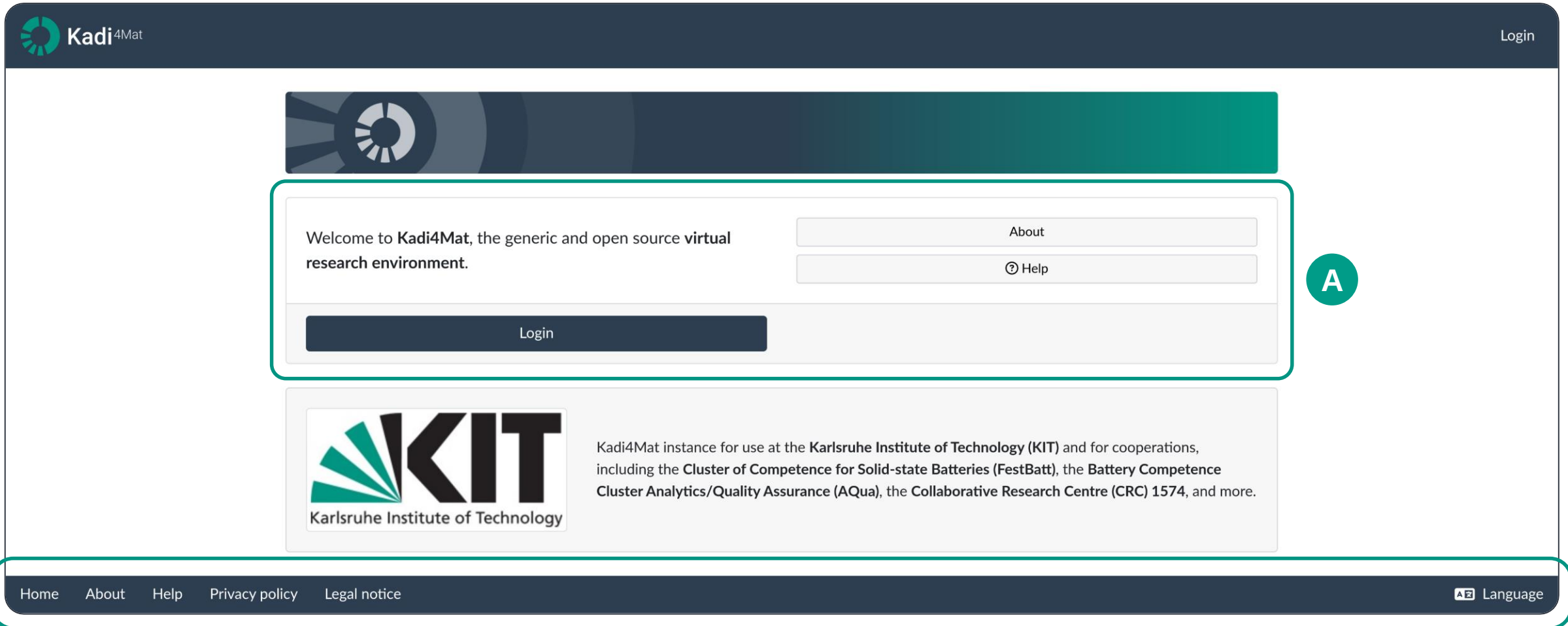
KadiAI ML Interface



The Graphical User Interface of Kadi4Mat

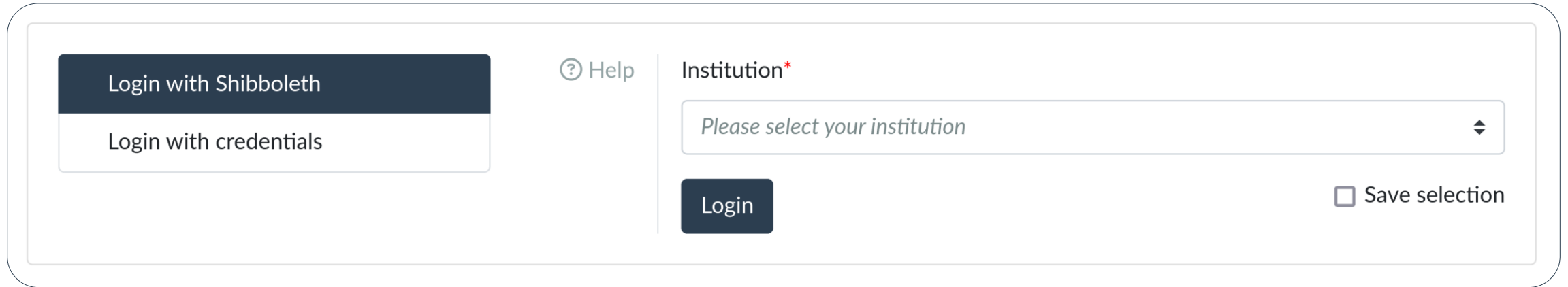
- The graphical user interface (GUI) is one of the main ways to use Kadi4Mat, and one of the easiest to get started with
- It can be used with all up-to-date web browsers and requires no additional software
- The REST-like HTTP API (Application Programming Interface) of Kadi4Mat exists next to the graphical user interface and enables programmatic usage of most functionality to facilitate automation and integration with existing programs and software

Kadi4Mat – Index Page



(A) Informational links and login (B) Navigation footer and language selection

Kadi4Mat – Login

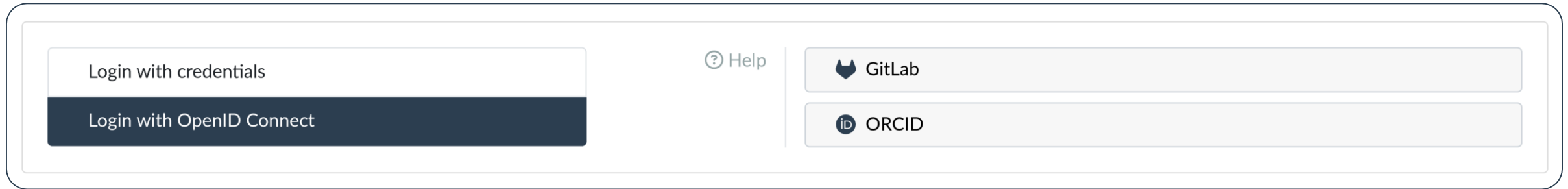


The login form is enclosed in a rounded rectangle. On the left, there is a vertical stack of two buttons: 'Login with Shibboleth' (dark blue) and 'Login with credentials' (light gray). To the right of these buttons is a small circular icon with a question mark and the text 'Help'. Further right is the label 'Institution*' in dark blue. Below this label is a dropdown menu with the placeholder text 'Please select your institution' and a small downward arrow icon. Below the dropdown is a dark blue 'Login' button. To the right of the 'Login' button is a checkbox labeled 'Save selection'.

- In our main Kadi4Mat instance, login is usually done using institutional accounts via **Shibboleth**
- If necessary (e.g. due to technical limitations), login via local accounts is also possible (accounts can be created manually by us on demand)
- Login scheme can be defined per instance



Kadi4Mat – OpenID Connect Integration



The screenshot shows a login interface for Kadi4Mat. On the left, there are two buttons: 'Login with credentials' and 'Login with OpenID Connect', with the latter being highlighted in dark blue. In the center, there is a 'Help' link with a question mark icon. On the right, there are two buttons for OpenID Connect providers: 'GitLab' (with a GitLab logo) and 'ORCID' (with an ORCID logo).

- Other instances may have different authentication providers, such as our public demo instance at <https://demo-kadi4mat.iam.kit.edu>, which also supports OpenID Connect and free registration of local accounts



Kadi4Mat – Home Page

Kadi4Mat Records Collections Templates Users Groups

Quick search

Recently visited

- DIN A4 Paper #001**
@din-a4-paper-001
Last visited 7 minutes ago
- Cutting Paper #001**
@cutting-paper-001
Last visited 10 minutes ago

Welcome to Kadi4Mat.
You are currently logged in as Nico Brandt.

Get started Hide

Start interactive tour

Check out the help page

The interactive tour will introduce the most important features of Kadi4Mat and is recommended in order to get started. More details and additional information can be found on the help page at any time.

Favorites View all

Record

Cutting Paper #001 experiment
@cutting-paper-001
No description.
Last modified a month ago

Record

DIN A4 Paper #001 sample
@din-a4-paper-001
A sheet of paper in DIN A4 format.
Last modified a month ago

Latest updates Configure

Records View all

(A) Navigation bar with links to the different resources and various menus/quick actions

(B) Favorited resources and latest updates (customizable)

Kadi4Mat – Interactive Tour

Get started

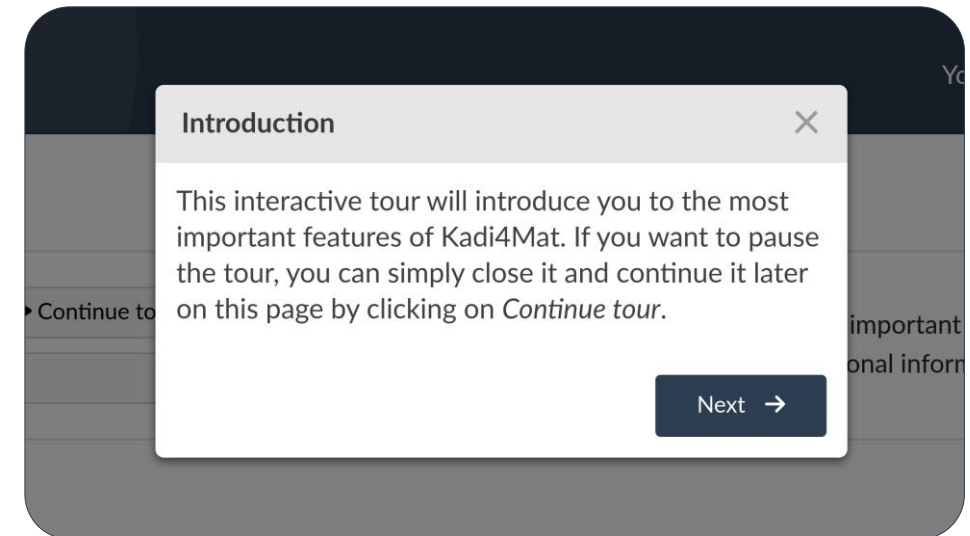
Hide

💡 Start interactive tour

❓ Check out the help page

The interactive tour will introduce the most important features of Kadi4Mat and is recommended in order to get started. More details and additional information can be found on the help page at any time.

- In addition to the help page, the interactive tour introduces some of the basic functionality of Kadi4Mat, with a focus on creating and managing records



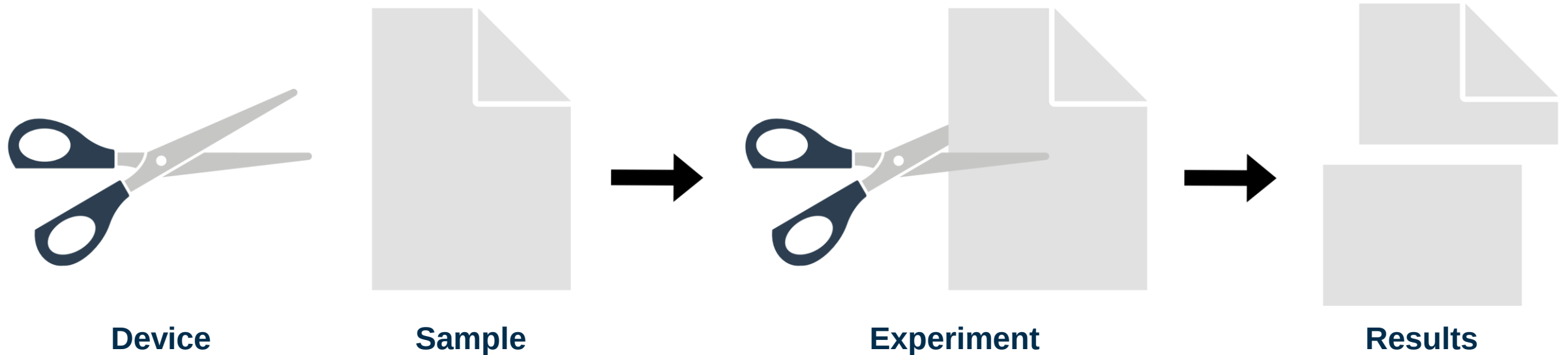
B

Kadi4Mat – Resources Overview



- **Records:** Basic components of Kadi4Mat, can represent any kind of digital or digitalized object via suitable metadata and/or corresponding data and can be linked together
- **Collections:** Represent logical groupings of multiple records (e.g. a single experiment) or other collections (e.g. a project with multiple experiment child-collections)
- **Templates:** Provide blueprints for either whole records, including record links and permissions, or just their generic metadata
- **Groups:** Group multiple users to facilitate permission management for different resources

Example Experiment Overview



→ All **inputs**, **processes** and **outputs** involved in the execution of the experiment can be represented as (metadata-only) records within Kadi4Mat (and optionally be grouped into a collection)

Example Experiment - Record of a Sample

DIN A4 Paper #001

sample

@din-a4-paper-001

Persistent ID: 40

A sheet of paper in **DIN A4** format.

Created by Nico Brandt

Created at August 21, 2024 9:02:29 AM (2 months ago)
Last modified at September 25, 2024 9:57:11 AM (a month ago)

License: Creative Commons Attribution 4.0 (CC-BY-4.0)

Tags:

paper

Generic Metadata
No (fixed) schema

Basic Metadata
Fixed schema

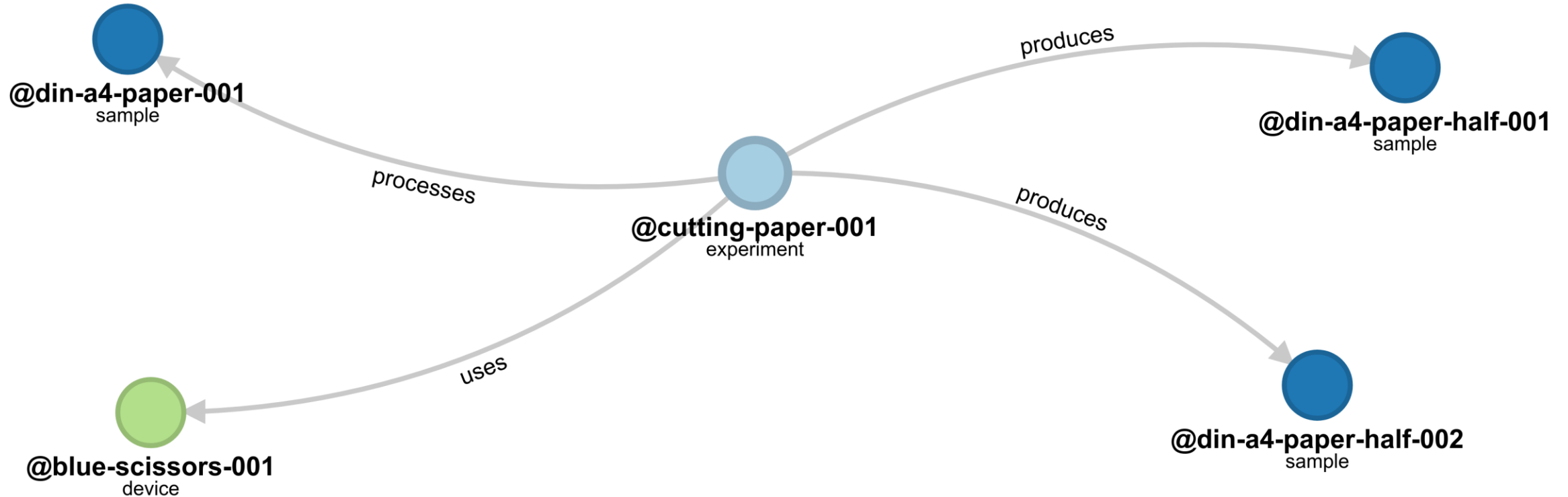
Extra metadata

-

+

Format	DIN A4	String	
Grammage	80 g/m²	Integer	
Measurements		Dictionary	
Width	210 mm	Integer	
Height	297 mm	Integer	

Example Experiment - Record Links and Data Provenance



- Record links can be seen as separate resources, with their own metadata (e.g. their name)
- They specify the **data provenance**, which creates a simplified version of a **knowledge graph**

Kadi4Mat – Creating New Record

Basic metadata

- Title
- (Unique) Identifier
- Type
- (Markdown) Description
- Tags
- License
- Visibility

Metadata

Title*

Identifier*

Unique identifier of this record.

Type

Enter or search for a record type

Optional type of this record, e.g. dataset, experimental device, etc.

Description

Preview

H B I S X¹ X₁ </> √* ⋮ ⋮ “ – ⌘ 🔗 🖼️ [] ↺ ↻

This editor supports Markdown, including math written in LaTeX syntax rendered with  KaTeX. Note that HTML tags and external images are not supported.

Tags

Enter or search for tags

An optional list of keywords further describing the record.

Kadi4Mat – Creating New Record

The screenshot shows the 'Extra metadata' editor in Kadi4Mat. At the top left, there is a toggle for 'Extra metadata'. To the right, there is a toolbar with icons for undo, redo, save, and refresh, followed by 'Simple mode' and 'Tree view' buttons. Below this, there are three rows of input fields. Each row has a 'Type' dropdown (currently set to 'String'), a 'Key' dropdown, a 'Value' dropdown, and a set of action buttons: '+', 'x', a document icon, and a list icon. At the bottom left, there is a '+ Add extra' button. At the bottom right, there is a 'Select a template' dropdown menu.

Generic metadata

- Enhanced and (potentially) nested key/value-pairs of different types
- Supports units for numeric values, basic validation instructions (depending on the type), custom descriptions and the specification of standardized metadata terms
- The corresponding editor has different modes and views to facilitate easier metadata entry and supports loading metadata from previously defined templates

Kadi4Mat – Generic Metadata Editor

^ Extra metadata

Type String

Key Sample string

Value* String value

Description

This is a sample string.

Term IRI

https://example.com#example

Find term

An IRI specifying an existing term that the metadatum should represent.

- While descriptions can provide a user-readable description of a metadatum, metadata terms are focused on machine readability and interoperability
- They enable the specification of identifiers (via Internationalized Resource Identifiers = IRIs), representing terms of existing metadata schemas/standards, vocabularies or ontologies

Kadi4Mat – Generic Metadata Term Search

Find term ×

Name ×

Class **Designative Name**
✎ <http://www.ontologyrepository.com/CommonCoreOntologies/DesignativeName>
A Designative Information Content Entity that consists of a string of characters that designates an entity within a specified cultural or social namespace and which is typically a word or phrase in a natural language that has an accepted cultural or social significance.

Class **Name**
✎ http://purl.obolibrary.org/obo/NCIT_C42614
The words or language units by which a thing is known.

Class **Name**
✎ <http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C42614>
The words or language units by which a thing is known.

Class **Name**
✎ http://emmo.info/domain-crystallography/cif_top#Name

Property **Name**
✎ <http://rs.tdwg.org/abcd/terms/name>
The name of a class in a specific language.

Note that these results are provided by an external terminology service.

« < Page 1 of 429 > »

 <https://terminology.tib.eu/ts>

TIB TERMINOLOGY SERVICE HOME COLLECTIONS ONTOLOGIES HELP API ABOUT

Name Search

Filter Results 4619 results found for "Name" Results Per Page 10

Clear All Filters

Type

- ☐ class 3642
- ☐ property 871
- ☐ individual 103
- ☐ ontology 3

Ontologies

- ☐ NCIT 2281
- ☐ EDAM 138
- ☐ MS 137
- ☐ FIBO 129
- ☐ ENM 110

+ Show More

Collections

- ☐ ESS
- ☐ NFDI4CHEM

Results:

[class] **Name** **NCIT_C42614**
http://purl.obolibrary.org/obo/NCIT_C42614
The words or language units by which a thing is known.
Ontology: NCIT

[class] **Name** **C42614**
<http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C42614>
The words or language units by which a thing is known.
Ontology: emm

[class] **Name** **Name**
<http://ecoinformatics.org/oboe/oboe.1.2/oboe-characteristics.owl#Name>
Ontology: oboe

[property] **name** **name**
<http://xmlns.com/foaf/0.1/name>

Terms can also be searched for using existing terminology services

Kadi4Mat – Creating New Record

Additional settings

Collections

Search for collections

Directly link this record with one or more collections.

Record links

Direction

Outgoing

Record

Search for records

Name

Enter or search for a name

+

Directly link this record with one or more other records.

Link preview

Permissions

Type

User

User

Search for users

Role

Member

+

Directly add user or group roles to this record.

Roles

- In addition to the metadata of the record itself (describing its content), additional settings can be specified while creating a record
- These include collections, record links and access permissions for users or groups

Kadi4Mat – File Import and Templates

Home / Records / New record

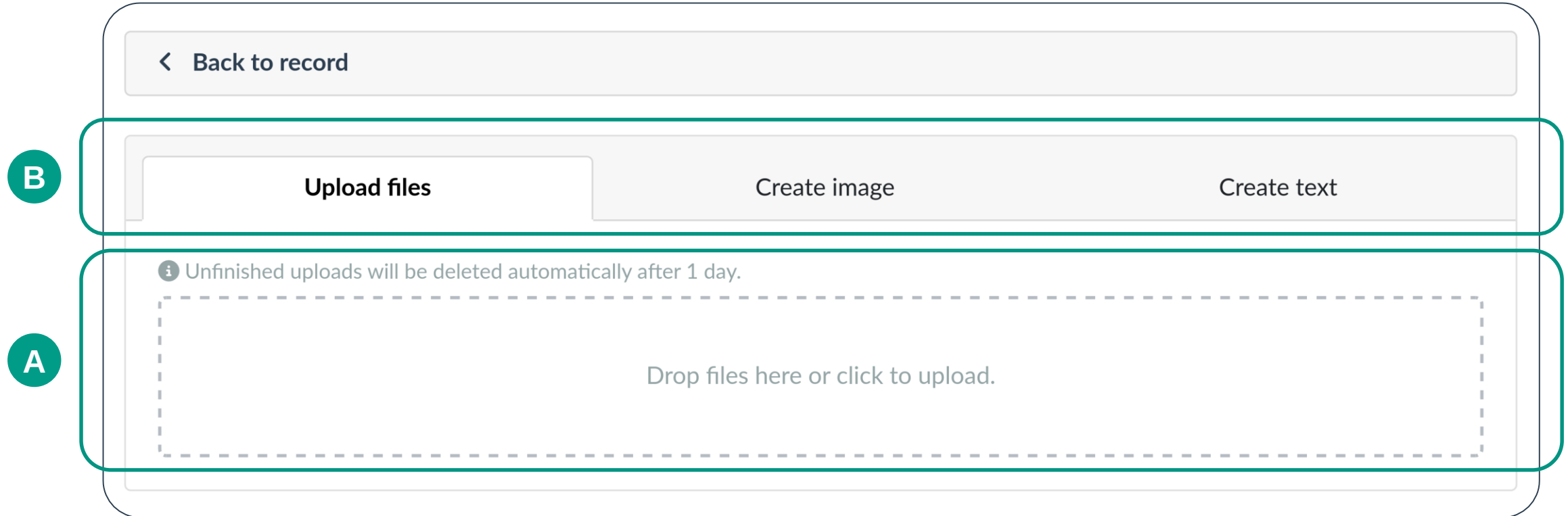
Import from file ▾ ? Help Select a record template ▾

Metadata

Title*

- When creating records, metadata and additional settings can also be imported from files (currently, only JSON files are supported within the GUI)
- In addition, previously defined (record) templates can be selected

Kadi4Mat – Adding Files to a Record



(A) Regular upload of local files

(B) Some file types can also be created (and edited) directly in the web interface

Kadi4Mat – Record Overview

The screenshot displays the 'Record Overview' page in Kadi4Mat. A teal box labeled 'A' highlights the top navigation bar, which includes tabs for 'Overview' (active), 'Files', 'Links', 'Permissions', and 'Revisions'. Another teal box labeled 'B' highlights the action bar below the tabs, containing buttons for 'Edit record', 'Copy record', 'As template', 'Export as', 'Publish via', and a star icon. The main content area shows a record titled 'DIN A4 Paper #001' with a lock icon, a 'sample' button, the identifier '@din-a4-paper-001', the 'Persistent ID: 40', and a description: 'A sheet of paper in DIN A4 format.'

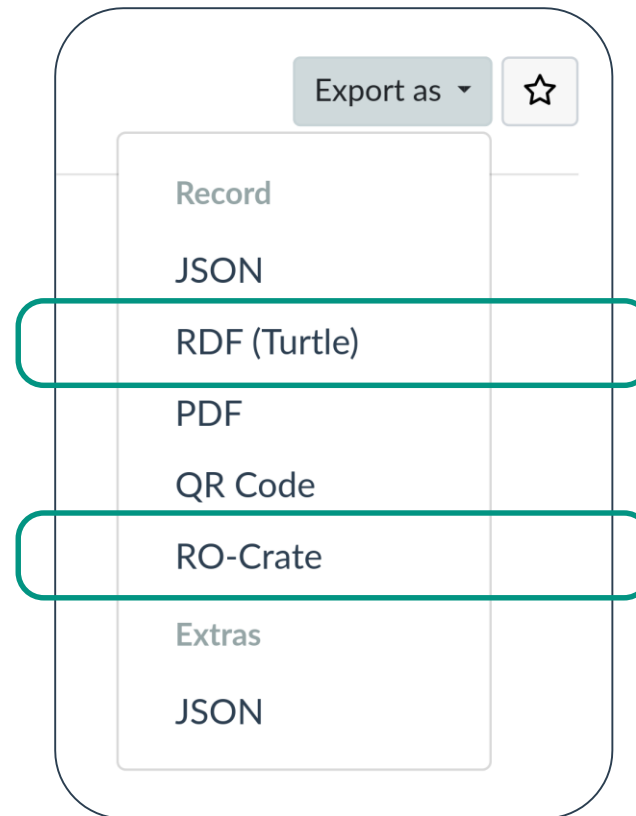
(A) Overviews of different contents of the record

(B) Additional (general and record-specific) actions, including exporting and publishing of records

Kadi4Mat – Export & Interoperability

- All relevant resource types in Kadi4Mat support exporting their (meta)data in different formats
- Exported data can be used for different purposes, including interoperability with other systems

Record export

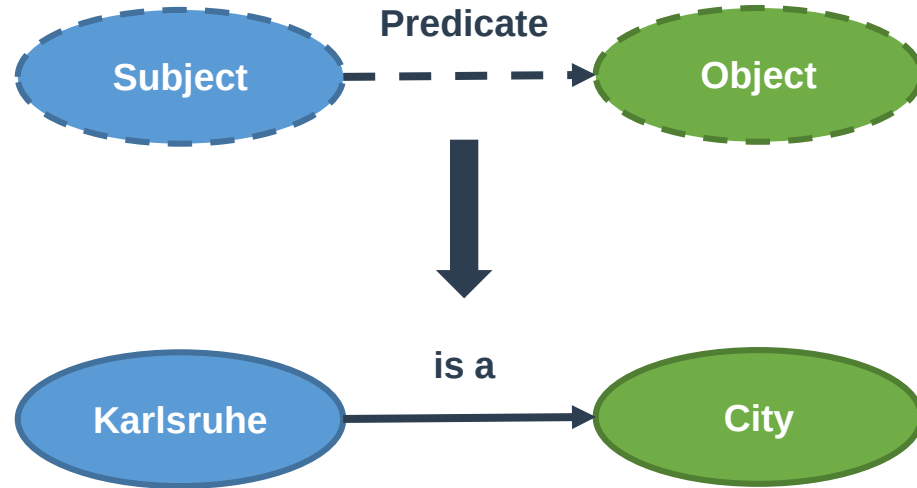


Template export



Kadi4Mat – RDF Export

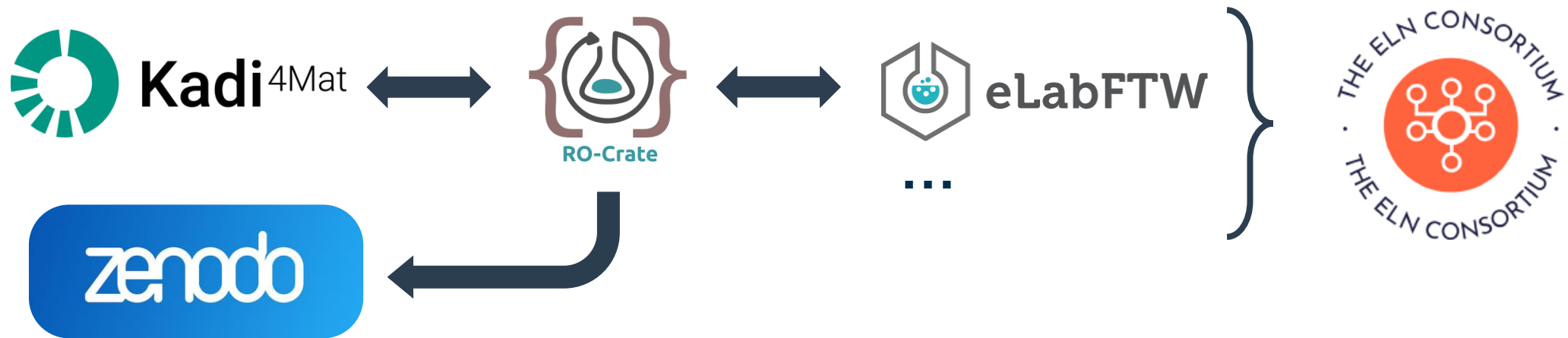
- Reminder: RDF (Resource Description Framework) is a standard for describing metadata in a graph and is the base of many ontology modelling languages
- Each graph is composed of triples specifying a **subject**, **predicate** and **object**
- Subjects, predicates and (optionally) objects make use of IRIs to describe the metadata in an interoperable manner (similar to the metadata term functionality from earlier)



```
<http://localhost:5000/records/40> a schema:Dataset ;  
  rdfs:isDefinedBy [ k4m40:Format "DIN A4" ;  
    k4m40:Grammage [ a schema:QuantitativeValue ;  
      schema:unitText "g/m²" ;  
      schema:value 80 ] ;  
    k4m40:Measurements [ k4m40:Height [ a schema:QuantitativeValue ;  
      schema:unitText "mm" ;
```

Kadi4Mat – RO-Create Export and Zenodo Publication

- RO-Crates are a container format for packaging research data and metadata of individual or multiple records (when exporting collections) in a ZIP file
- They are also used as container when publishing resources to **Zenodo** via Kadi4Mat
- Furthermore, various different ELN-like systems are collaborating to establish RO-Crate as a means of exporting/importing data in an interoperable manner as part of the ELN Consortium [1]



[1] <https://github.com/theelnconsortium>

Kadi4Mat – File Overview

A

Overview Files Links Permissions Revisions

Add files Download all

Files 1 Sort by Last modified (newest first)

01_Introduction.pdf application/pdf 1.1 MB

Last modified a minute ago Edit file Update data Delete Download

Filter

(A) Adding new or downloading existing files

Kadi4Mat – File Metadata and Preview

A

Edit file **Update data** **Download**

01_Introduction.pdf application/pdf **Storage type: Local**

1.1 MB **28e0040058ac5fb6bbf1253bd6605a43**

Persistent ID: 3f6a6aeb-f6f3-423b-a829-e31b4a41533a

No description.

Created by User Created at January 17, 2025 10:46:00 AM (a few seconds ago)
Last modified at January 17, 2025 10:46:00 AM (a few seconds ago)

4 of 14 Automatic Zoom

Research Data Management (RDM)

Plan

(A) Editing the file metadata or updating its data (potentially directly in the web interface, if supported)

Kadi4Mat – Linked Resources Overview

A

Overview Files **Links** Permissions Revisions

Manage links Visualize record links

Outgoing record links 0

No record links.

Incoming record links 1

processes

Cutting Paper #001 experiment

@cutting-paper-001

Last modified 4 months ago

View record Edit link

Filter

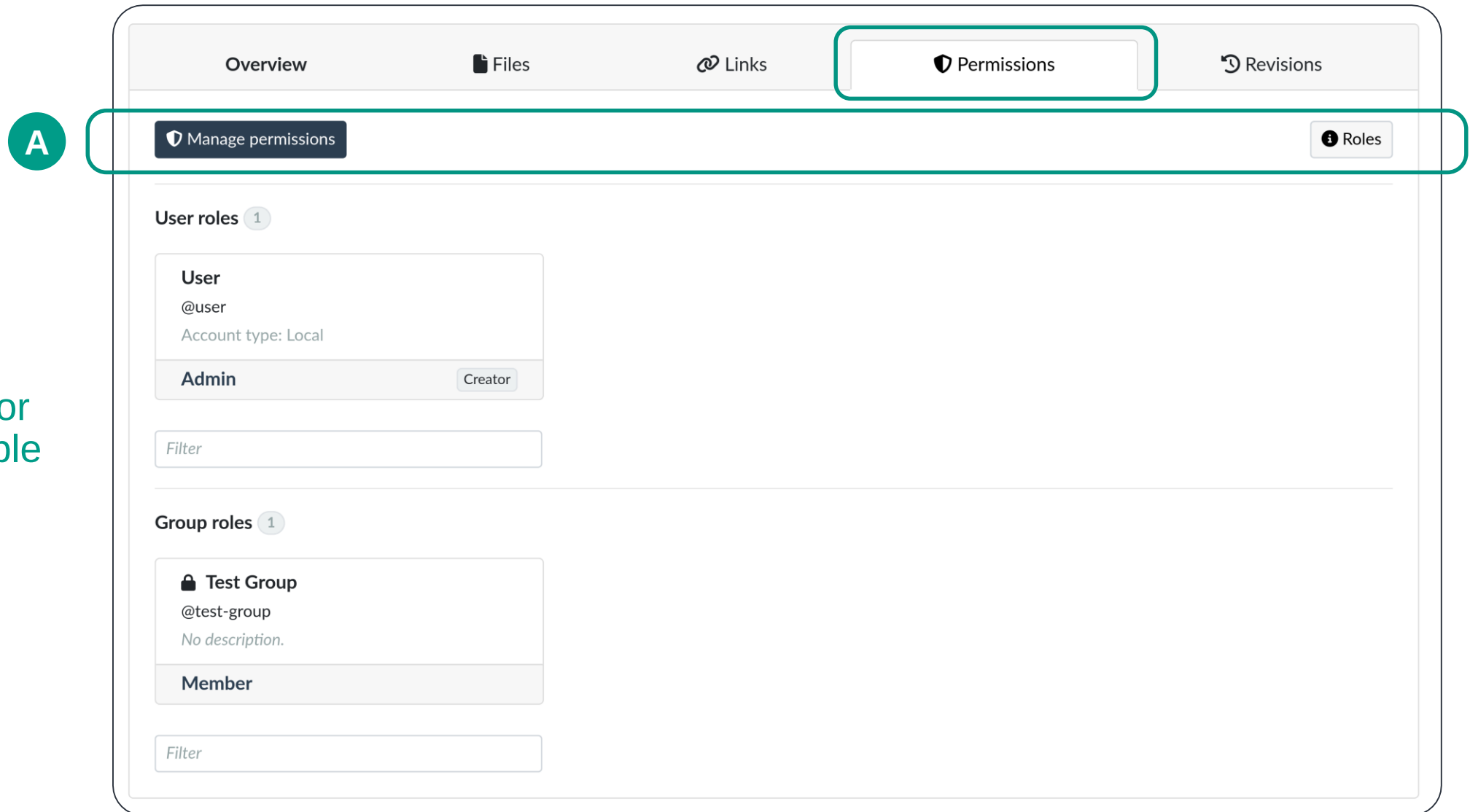
Collections 0

No collections.

(A) Managing linked resources (record links and collections) or visualizing record links (as seen previously)

Kadi4Mat – Permission Overview

(A) Managing user/group roles or displaying available roles



Kadi4Mat – Revision Overview

Overview

Files

Links

Permissions

Revisions

Record revisions 2

 User updated DIN A4 Paper #001

4 months ago

 View revision

 User created DIN A4 Paper #001

5 months ago

 View revision

File revisions 1

 User created 01_Introduction.pdf

a minute ago

 View revision

- Records include both record revisions, for record metadata and record link data, revisions of corresponding files
- Note that file revisions currently only include the file metadata

Kadi4Mat – Record Search

(A) Searching of basic (title, identifier, description) or generic record metadata

(B) Further filtering of results via different attributes and management of saved search filters

The screenshot shows the Kadi4Mat Record Search interface. A teal box labeled 'A' highlights the top search bar area, which includes a 'Help' button, a 'Type' dropdown, a 'Key' input field, a quote icon, and a '+' button. Below this is a search input field with the placeholder text 'Search title, identifier and description', a magnifying glass icon, a 'Search' button, a 'Sort by' dropdown set to 'Relevance', and an 'Extras' button. A dark blue button labeled 'Create new record' is positioned below the search bar. A second teal box labeled 'B' highlights the left sidebar, which contains a 'Select a saved search' dropdown with a '+' button, a 'Toggle filters' button, a 'Results per page: 10' section with a slider from 10 to 100, a 'Filter by visibility' dropdown set to 'All', and a checkbox for 'Only consider explicit permissions'. The main content area on the right shows '35 results found' and lists three records: 'DIN A4 Paper #001' (sample), 'Sample record 12' (sample), and 'Test Extras'. Each record entry includes the record name, a sample label, the user who created it, the creation and modification dates, and a description. A 'Toggle filters' button is located above the first record. Each record entry also has a 'Toggle filters' button and a 'Extra metadata' link.

Home / Records

Help Type Key " +

Search title, identifier and description " Search Sort by Relevance ^ Extras

Create new record

Select a saved search +

^ Toggle filters

Results per page: 10

10 100

Filter by visibility

All

☐ Only consider explicit permissions

35 results found

DIN A4 Paper #001 sample Created 5 months ago
@din-a4-paper-001 Last modified 4 days ago

A sheet of paper in DIN A4 format.

Created by User ^ Extra metadata

Sample record 12 sample Created a year ago
@sample-record-12 Last modified 8 days ago

This is a sample record. New line. Another test New line

Created by User ^ Extra metadata

Test Extras Created 10 months ago
@test-extras Last modified 13 days ago

No description.

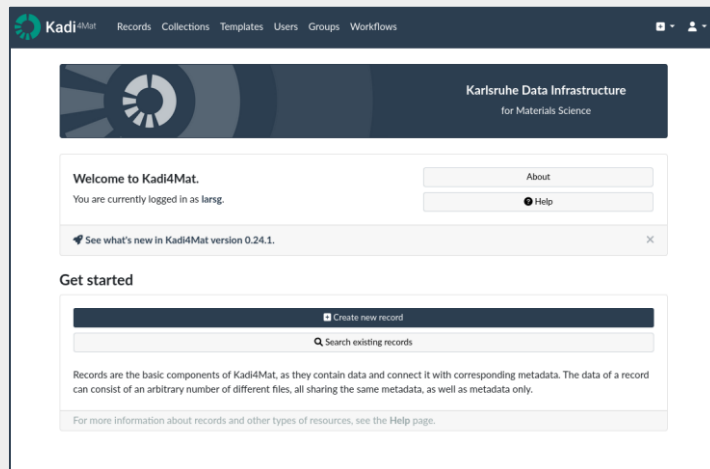
Created by User ^ Extra metadata

KadiAI and CIDS

3

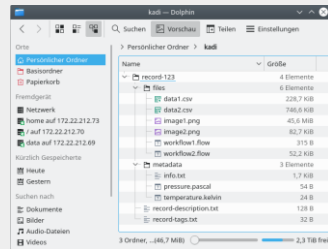
The Kadi Ecosystem

KadiWeb Repository / Web



KadiFS

Filesystem



Streamline your research

KadiStudio

Workflows



KadiAPY

(Python) API

```

kali@kali:~$ sudo systemctl status kodi.service
● kodi.service - Kodi media center
   Loaded: loaded (/lib/systemd/system/kodi.service; vendor preset: enabled)
   Active: active (running) since 2018-07-27 12:00:00; 1min 10s ago
     Main PID: 1000 (kodi)
    CGroup: /systemd/system/kodi.service
            └─ 1000 kodi

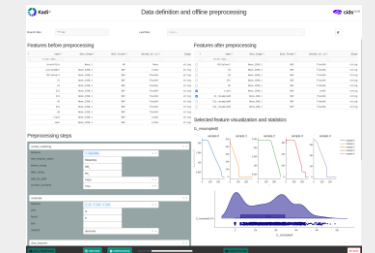
kali@kali:~$ systemctl restart kodi.service
kali@kali:~$ systemctl status kodi.service
● kodi.service - Kodi media center
   Loaded: loaded (/lib/systemd/system/kodi.service; vendor preset: enabled)
   Active: active (running) since 2018-07-27 12:00:00; 1min 10s ago
     Main PID: 1000 (kodi)
    CGroup: /systemd/system/kodi.service
            └─ 1000 kodi

kali@kali:~$ systemctl stop kodi.service
kali@kali:~$ systemctl status kodi.service
● kodi.service - Kodi media center
   Loaded: loaded (/lib/systemd/system/kodi.service; vendor preset: enabled)
   Active: inactive (dead) since 2018-07-27 12:00:00; 1min 10s ago
     Main PID: 1000 (kodi)
    CGroup: /systemd/system/kodi.service
            └─ 1000 kodi

```

KadiAI

ML Interface



KadiAI and CIDS



Kadi Artificial Intelligence

- MLOps: Standardized AI projects and workflows integrated into Kadi
- Reproducible and comparable results
- Data provenance tailored to AI applications
- Interactive definition of the data, model, and training using dashboards

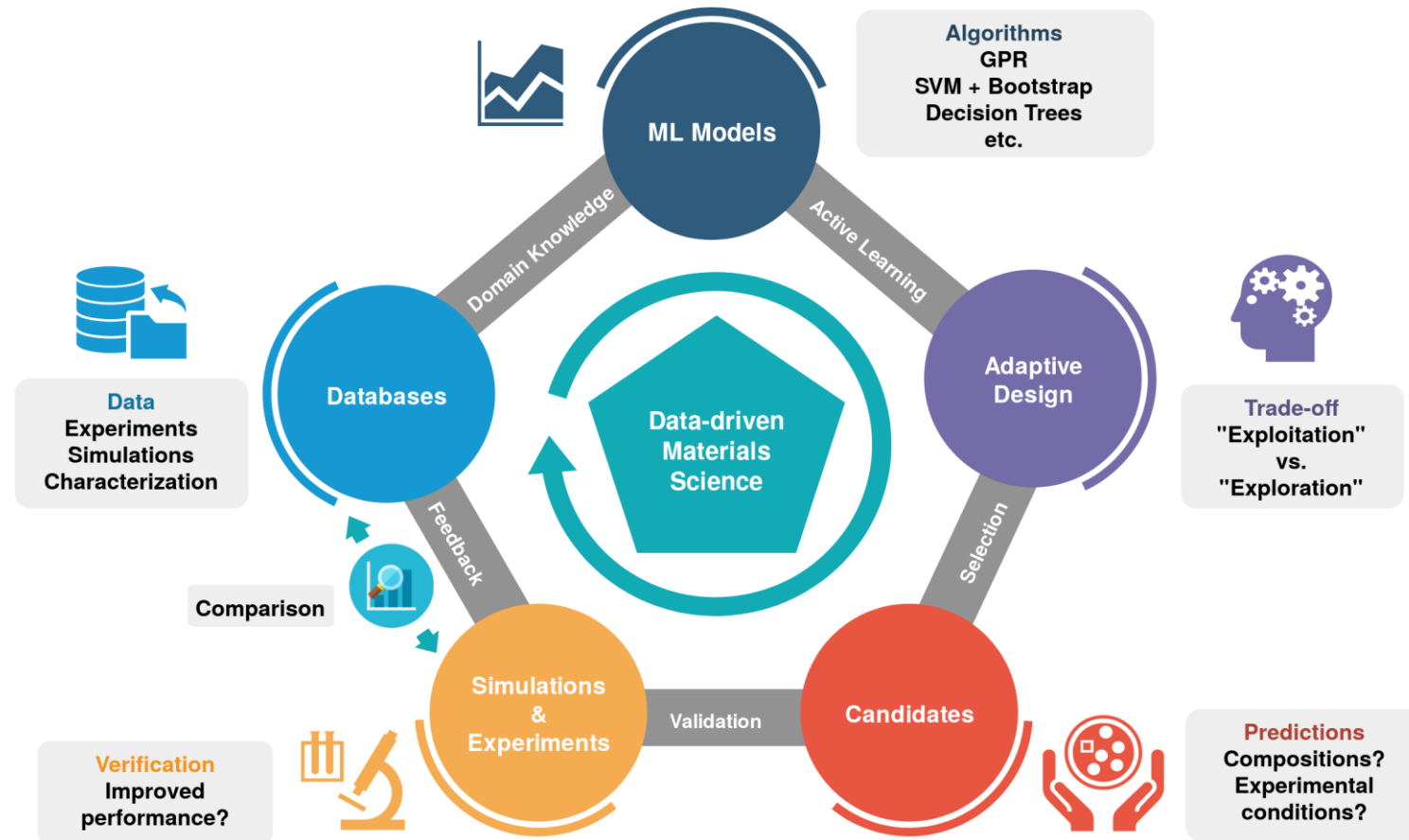


Computational Intelligence and Data Science

- Python framework for AI methods in the STEM sciences
 - Based on Tensorflow/Keras, SciKit-Learn, and SciPy (More to come...)
 - Python script and Jupyter notebooks
- Workflow nodes for Kadi's workflow engine KadiStudio
- Development and standardization of machine learning code

Data-integrated Artificial Intelligence

- Repositories to store and describe data
- Workflows for reproducible simulations, experiments and analyses
- Standardized yet customizable AI models
- AI models and machine learning needs to interact with repository and workflows
 - AI-driven design
 - Active Learning

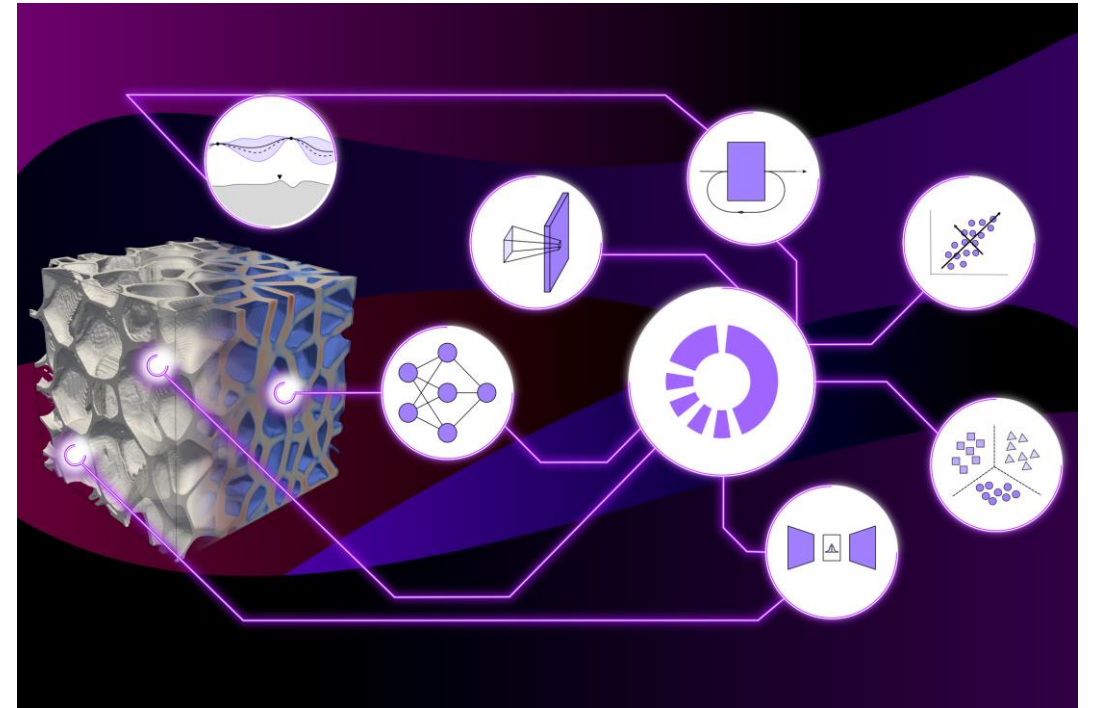


Data-integrated AI for Systematic Parameter Exploration

- Many studies that involve data or statistics (e.g., in engineering or natural sciences) **investigate parameter spaces** based on performance metrics or objective functions
- Most of these studies have explorative or exploitative characteristics
 - Mapping of parameter sensitivity (e.g., computational benchmarks, clinical trials)
 - Discovery of new materials (e.g., new electrolytes)
 - Optimizing processes or experimental settings (e.g., optimal amount of additives, cost minimization)

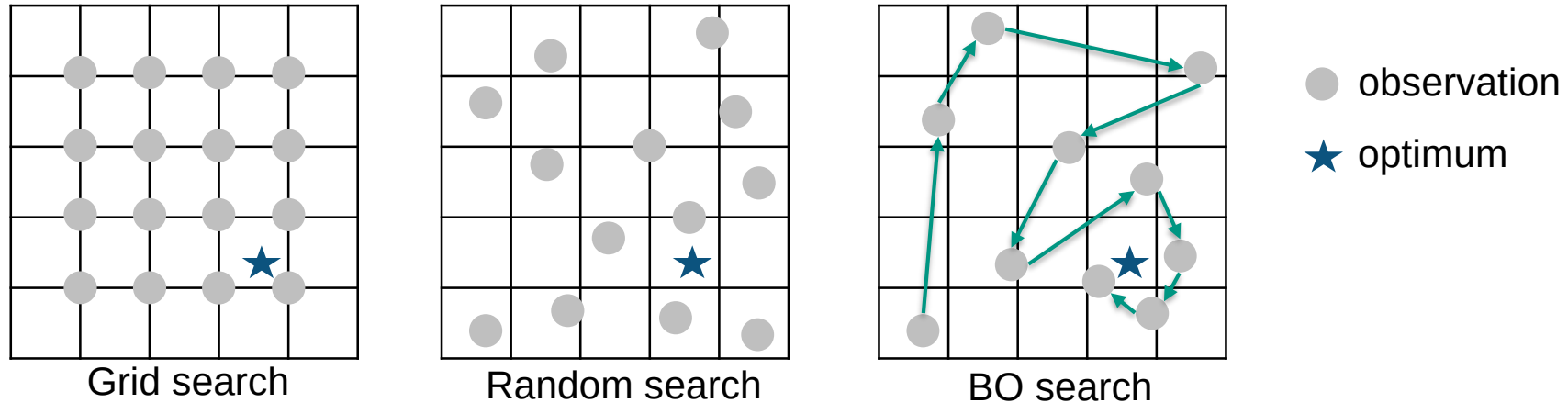
Data-driven modeling / statistics / Machine Learning (ML) / Artificial Intelligence (AI) **aims to accelerate these kind of investigations**

- KadiAgent plugins and FINALES tenants



Method: Active Learning

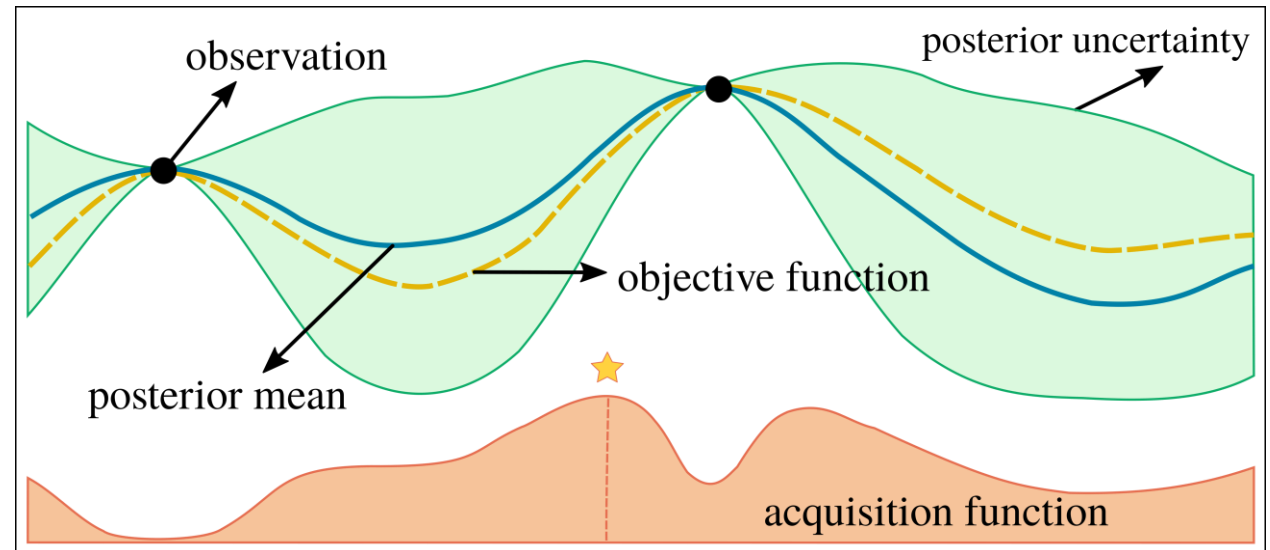
- Investigation strategies for global optimization of black-box functions (Design-of-experiments)
 - Sequential: Bayesian Optimization (BO)
 - More efficient than grid search or random sampling (terms and conditions apply)



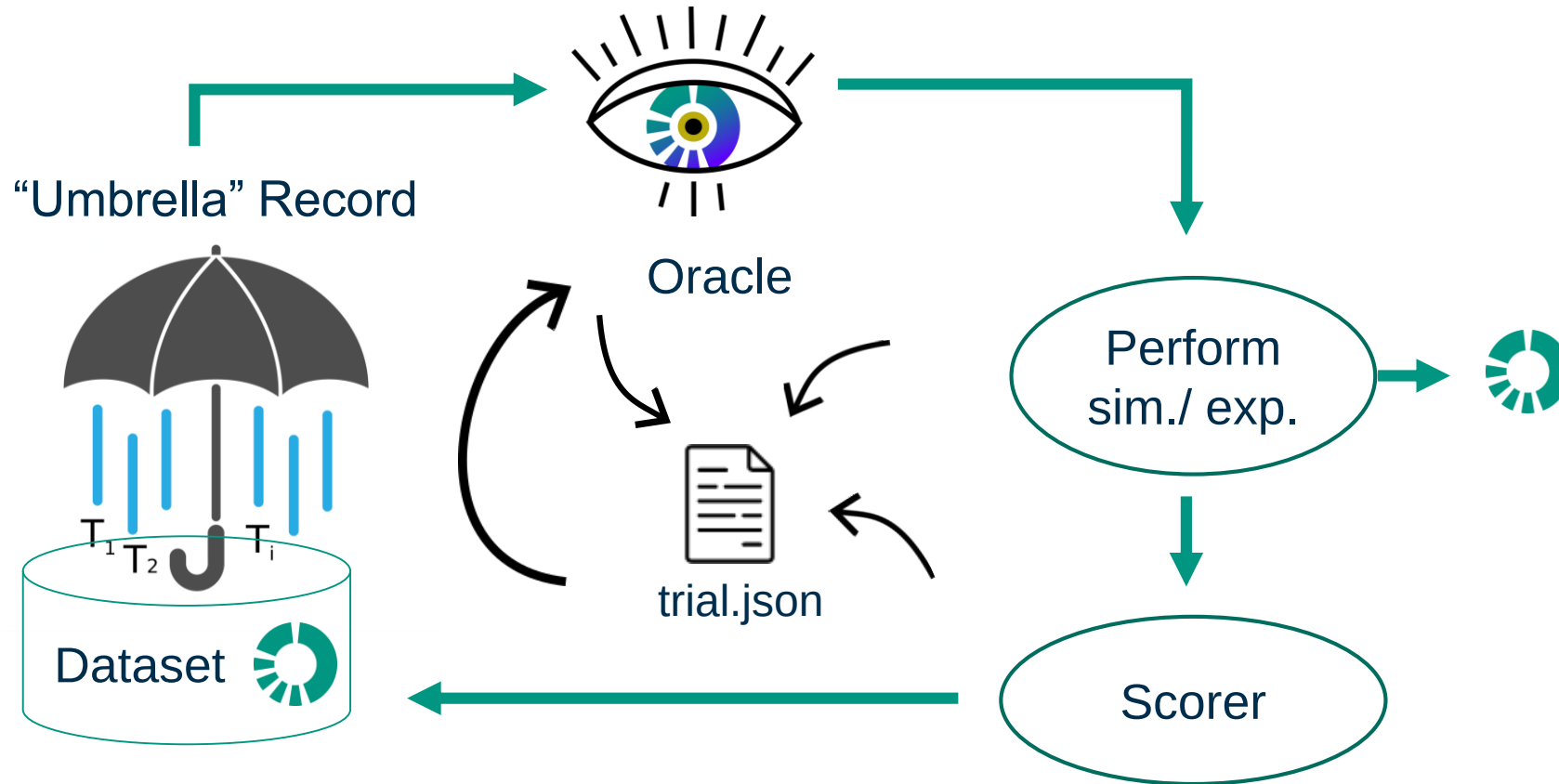
- Advantages
 - Predict promising configuration / candidates
 - Reduce required time for experimental / numerical studies

Bayesian Optimization

- Find the most informative new data point guided by previous evaluations
- Prediction with uncertainty
- Surrogate model
 - Gaussian Process
 - Incorporate the belief on the objective
 - Quantifies the uncertainty in form of a posterior distribution



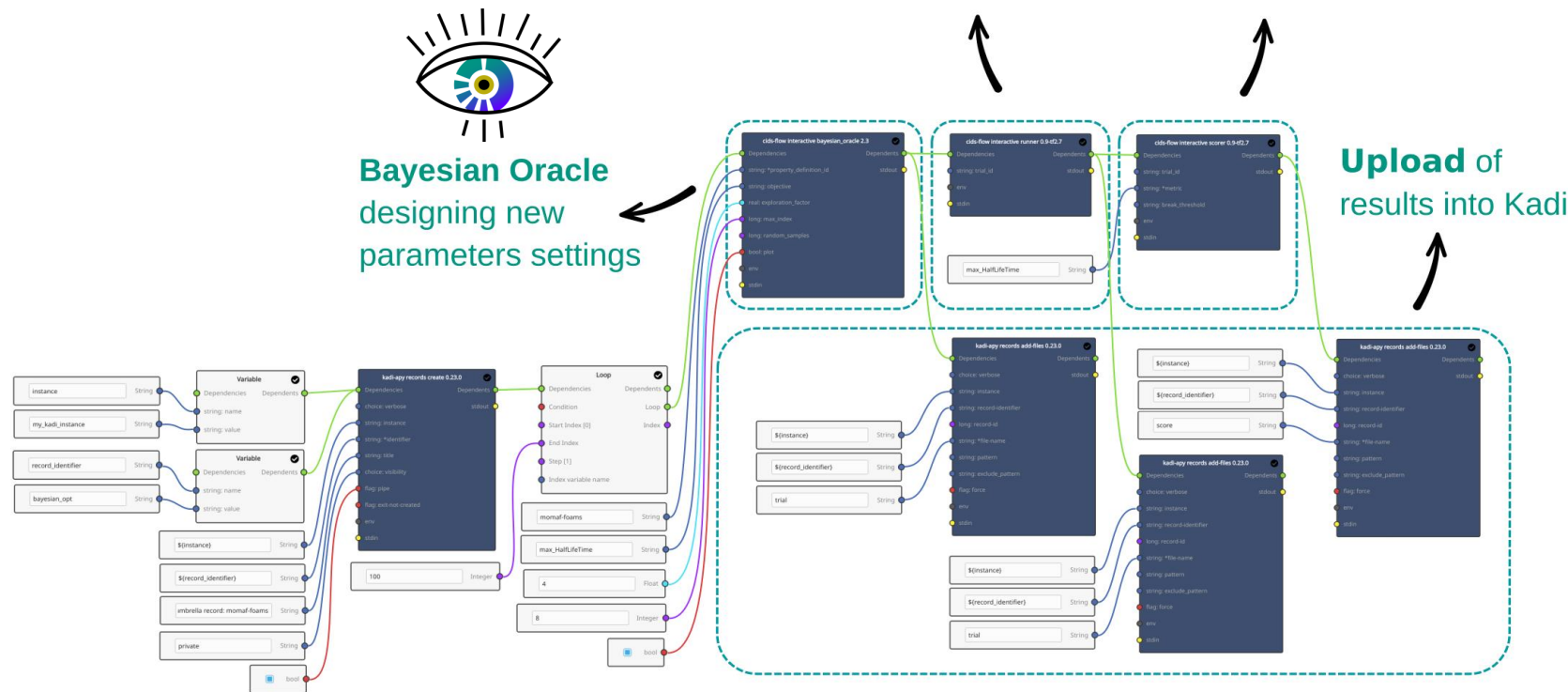
Active Learning Oracle Schema



Active Learning in KadiStudio

Oracle workflow node

- Perform Bayesian optimization in KadiStudio and link Records in Kadi4Mat repository



Tools and Use Cases

4

Model Parametrization for Solid Oxide Fuel Cells

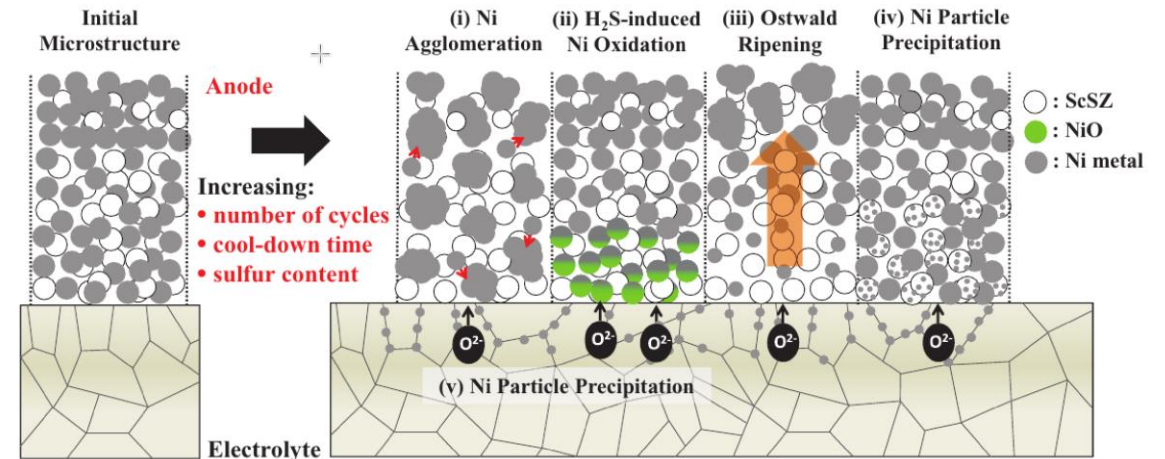
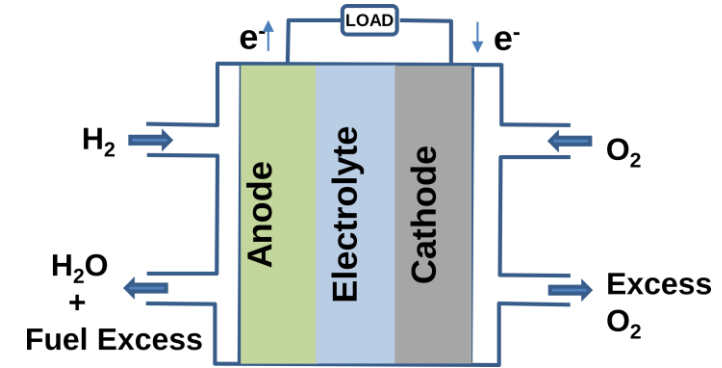
■ Solid Oxide Fuel Cell (SOFC)

- High efficiency & fuel flexibility
- Operating temperature 750°C – 1000°C
- Key micro. properties: TPB density, effective conductivity, specific surface area...

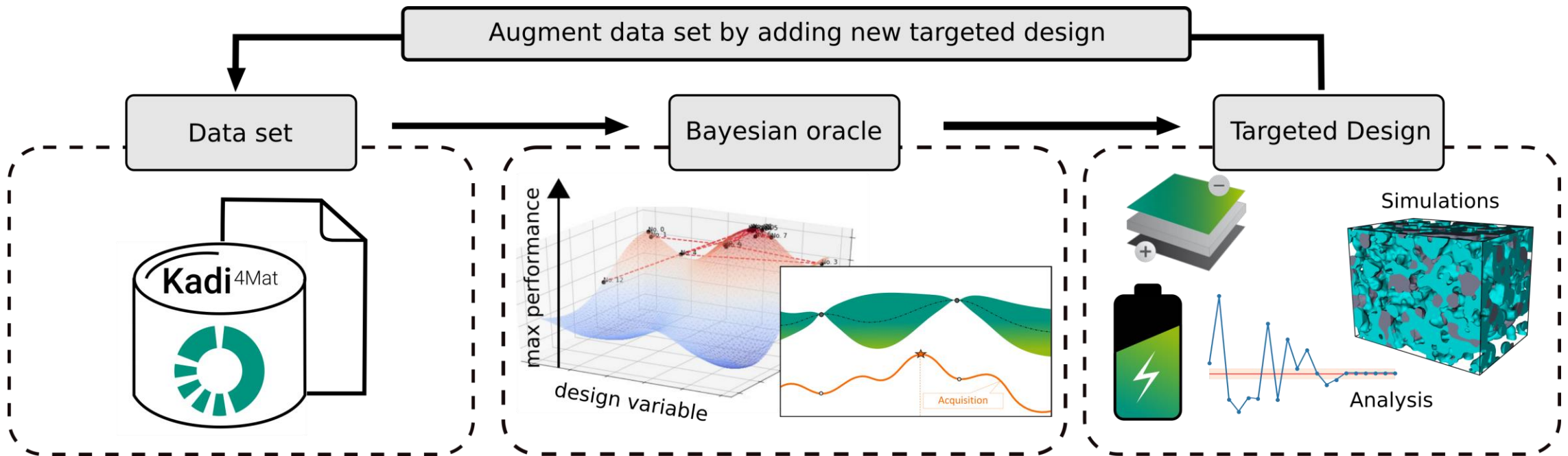
■ Degradation

- Microstructural changes within SOFC anode functional layer
- Coarsening

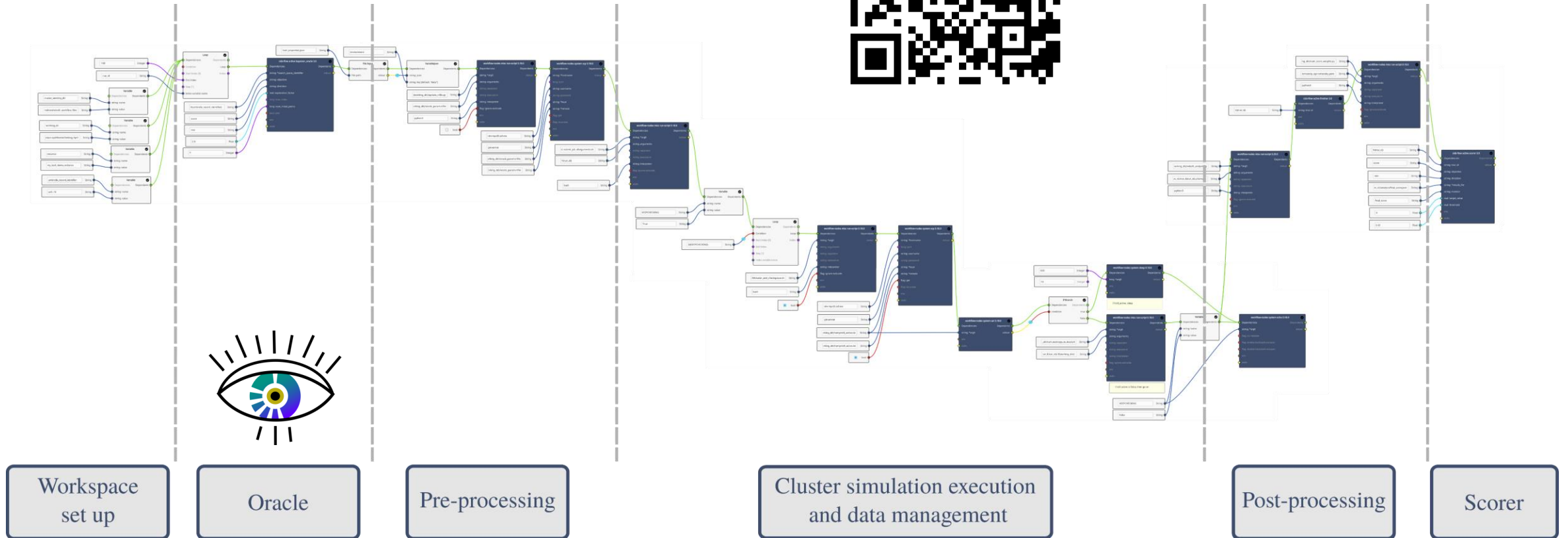
■ Ni/GDC vs. Ni/YSZ



Active Learning Bayesian Optimization – Framework Integration



KadiStudio Workflow



Workspace – Umbrella Record in KadiWeb

Kadi4Mat
Records
Collections
Templates
Users
Groups

+

Quick search

?

Overview

Files

Links

Permissions

Revisions

Edit record

Copy record

As template

Export as

Publish via

☆

Enhancing Solid Oxide Fuel Cells Development through Bayesian Active Learning

umbrella

@enhancing-sofcs-through-al

Persistent ID: 42014

Umbrella record for 7-dim parameter study of Ni/GDC anode in Soli (scalarization approach).

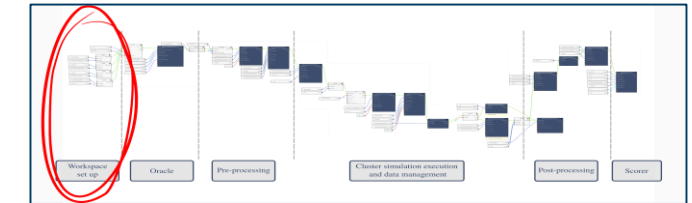
Extra metadata

g_ni_gdc

min	0.4
max	1.2
step	0.01

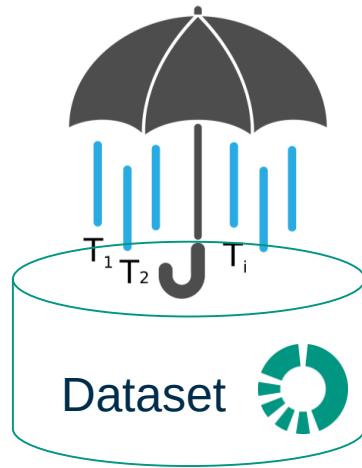
g_pore_gdc

min	0.28
max	0.8
step	0.01



Parameter (symbol)	Value (model units)	Value (physical units)
Interfacial energy Ni-GDC (γ_{NiGDC})	$1.2 \dots 0.4 \, u_E / u_l^2$	$3.0 \dots 1.0 \, \text{J m}^{-2}$
Interfacial energy Pore-GDC (γ_{GDCPore})	$0.8 \dots 0.28 \, u_E / u_l^2$	$2.0 \dots 0.7 \, \text{J m}^{-2}$
Interfacial energy Ni-Pore (γ_{NiPore})	$1.0 \dots 0.6 \, u_E / u_l^2$	$2.5 \dots 1.5 \, \text{J m}^{-2}$
Diff. coeff. GDC-surf. ($M_{\text{GDC}}^{\text{GDCPore}}$)	$(2.11 \times 10^{-6} \dots 2.11 \times 10^{-9}) \, u_l^6 / (u_E u_l)$	$(3.65 \times 10^{-34} \dots 3.65 \times 10^{-37}) \, \text{m}^6 / \text{J/s}$
Diff. coeff. GDC-nickel/GDC interf. ($M_{\text{GDC}}^{\text{NiGDC}}$)	$(2.11 \times 10^{-8} \dots 2.11 \times 10^{-14}) \, u_l^6 / (u_E u_l)$	$(3.65 \times 10^{-36} \dots 3.65 \times 10^{-42}) \, \text{m}^6 / \text{J/s}$
Diff. coeff. Ni-nickel/GDC interf. ($M_{\text{Ni}}^{\text{NiGDC}}$)	$(10^{-3} \dots 10^{-8}) \, u_l^6 / (u_E u_l)$	$(1.73 \times 10^{-31} \dots 1.73 \times 10^{-36}) \, \text{m}^6 / \text{J/s}$
Diff. coeff. Ni-surf. ($M_{\text{Ni}}^{\text{NiPore}}$)	$(10^{-1} \dots 10^{-3}) \, u_l^6 / (u_E u_l)$	$(1.73 \times 10^{-29} \dots 1.73 \times 10^{-31}) \, \text{m}^6 / \text{J/s}$

Active Learning Oracle



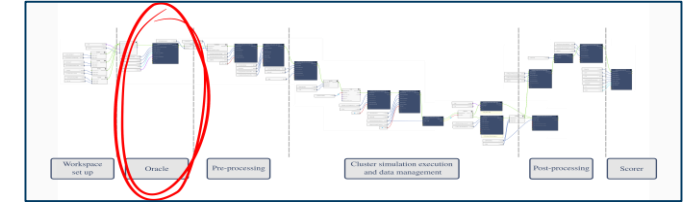
Model

Query
Selection

**Active
Learning
(Bayesian Opt.)**

Evaluation

Oracle



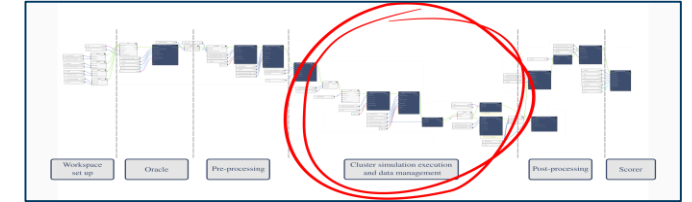
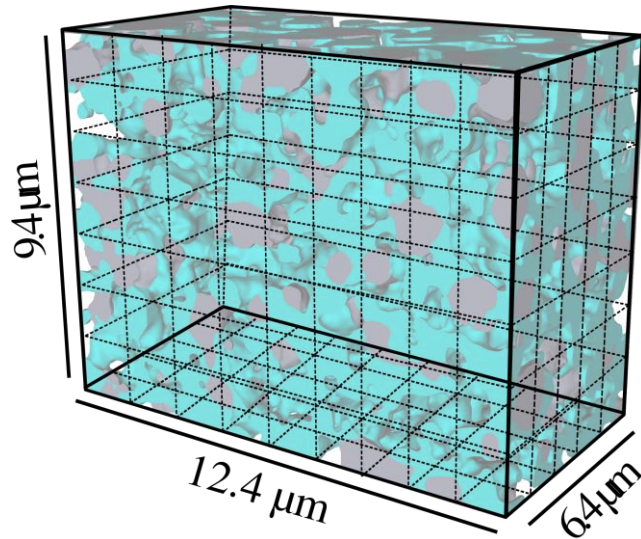
Pre-processing and Data Management

- KadiStudio allows to integrate:
 - Experimental devices
 - Numerical methods
 - Pre-built tool nodes
 - Customizable functions
- For the AL framework:
 - Conversion of Oracle output information into simulation inputs



HPC-Cluster (idm-hpc03)

- 8 computing nodes
- Each node equipped with two AMD EPYC™ 7452 processors
- 64 cores per node (32 cores per processor)
- Interconnect: via 100 Gbit/s InfiniBand network
- Job Scheduler: SLURM

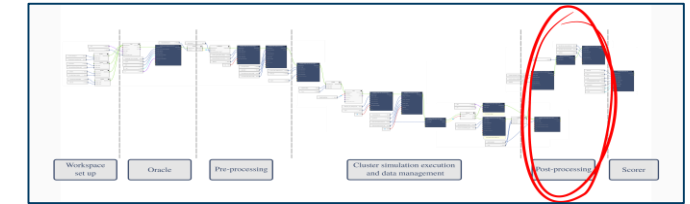
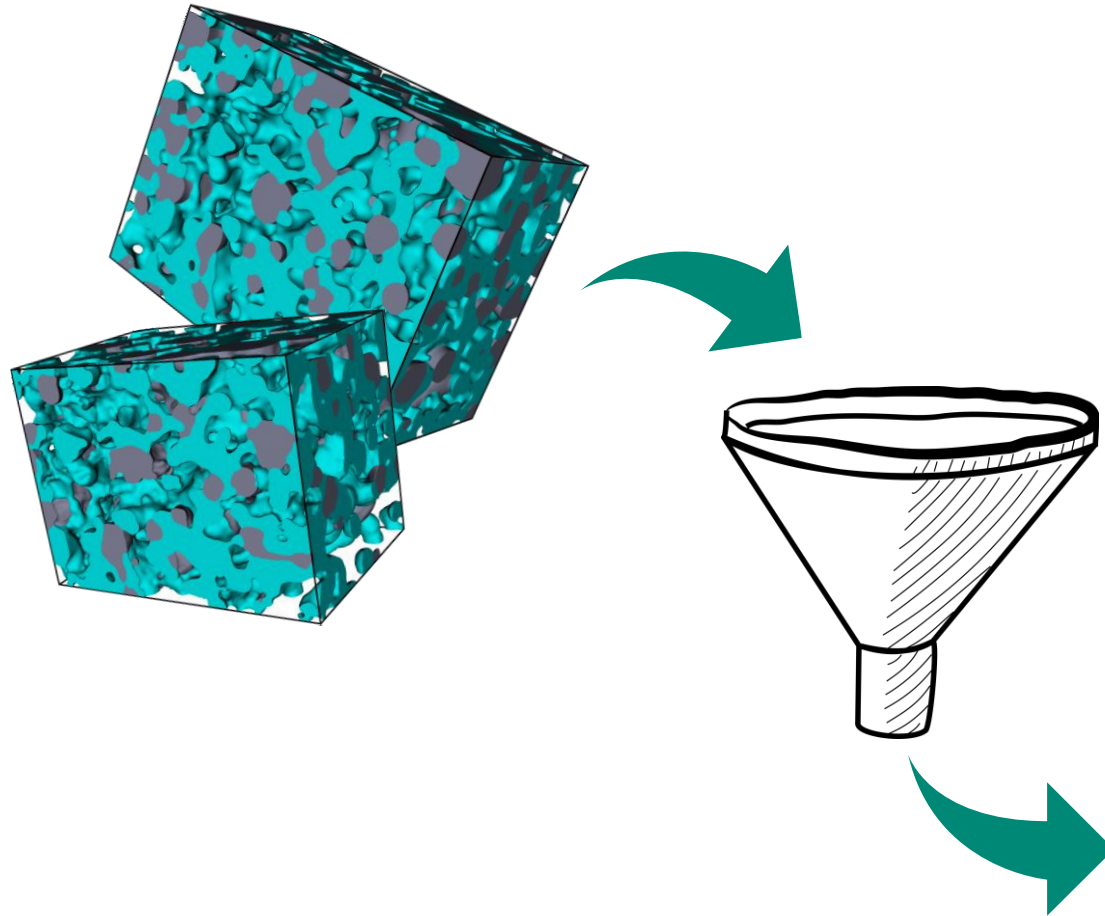


- For our study:

Domain decomposition
partition: (7, 9, 5)

#SBATCH -n 315

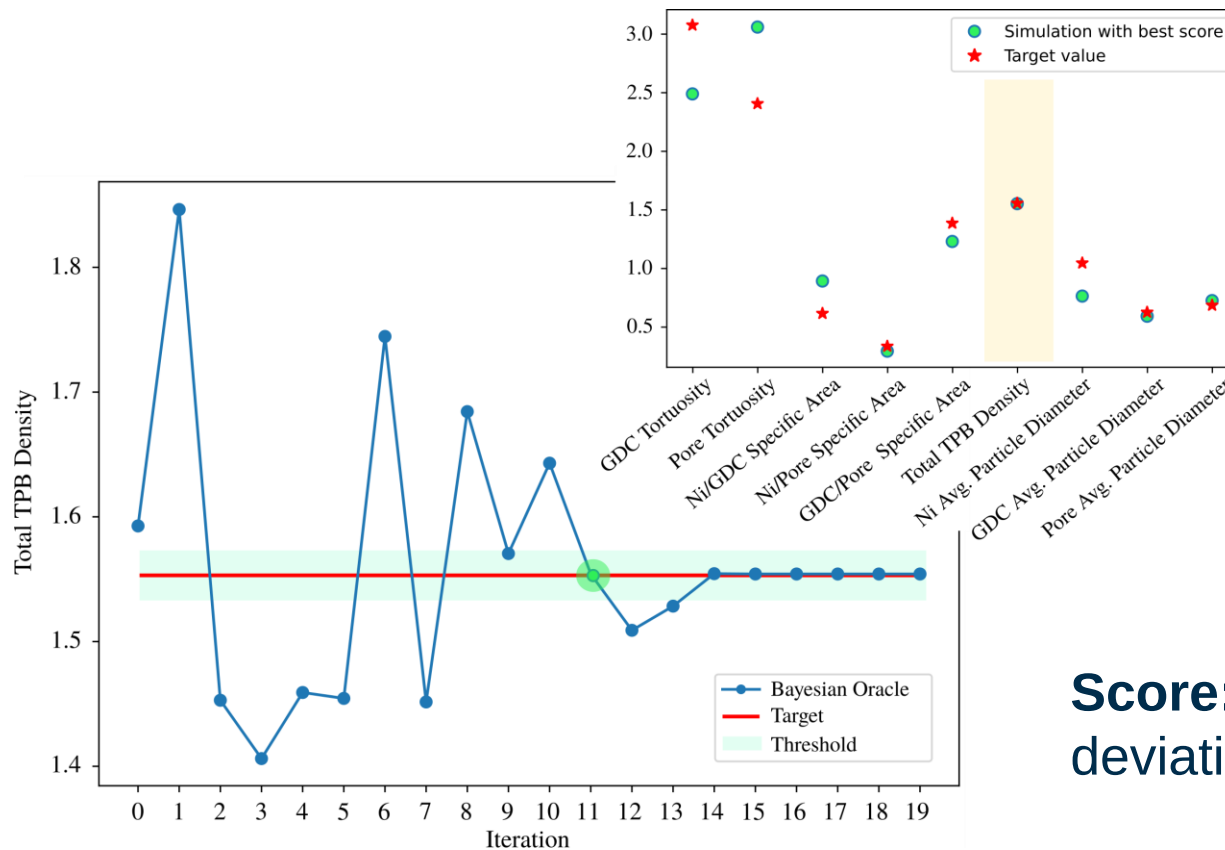
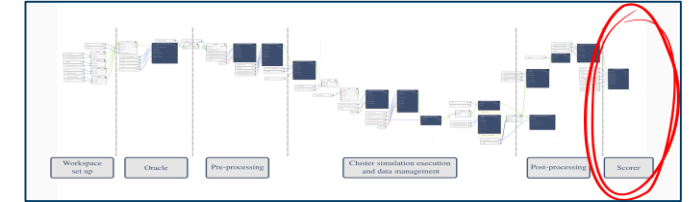
Post-processing



GDC Tortuosity	3.2e-3
Pore Tortuosity	9.8e-4
Ni/GDC Specific Area	7.9e-5
Ni/Pore Specific Area	7.5e-4
GDC/Pore Specific Area	3.3e-5
Total TPB Density	5.2e-4
Ni Avg. Particle Diameter	6.0e-4
GDC Avg. Particle Diameter.	1.5e-7
Pore Avg. Particle Diameter.	2.5e-5

Scoring System (naive)

- Single objective optimization: one microstructural property as objective as objective



Score: Triple Phase Boundary Density deviation

Scoring System – Scalarization Approach

- (Degenerative) multi-objective optimization

$$F(x) = w_1 * f_1(x) + w_2 * f_2(x) + \dots + w_n * f_n(x)$$

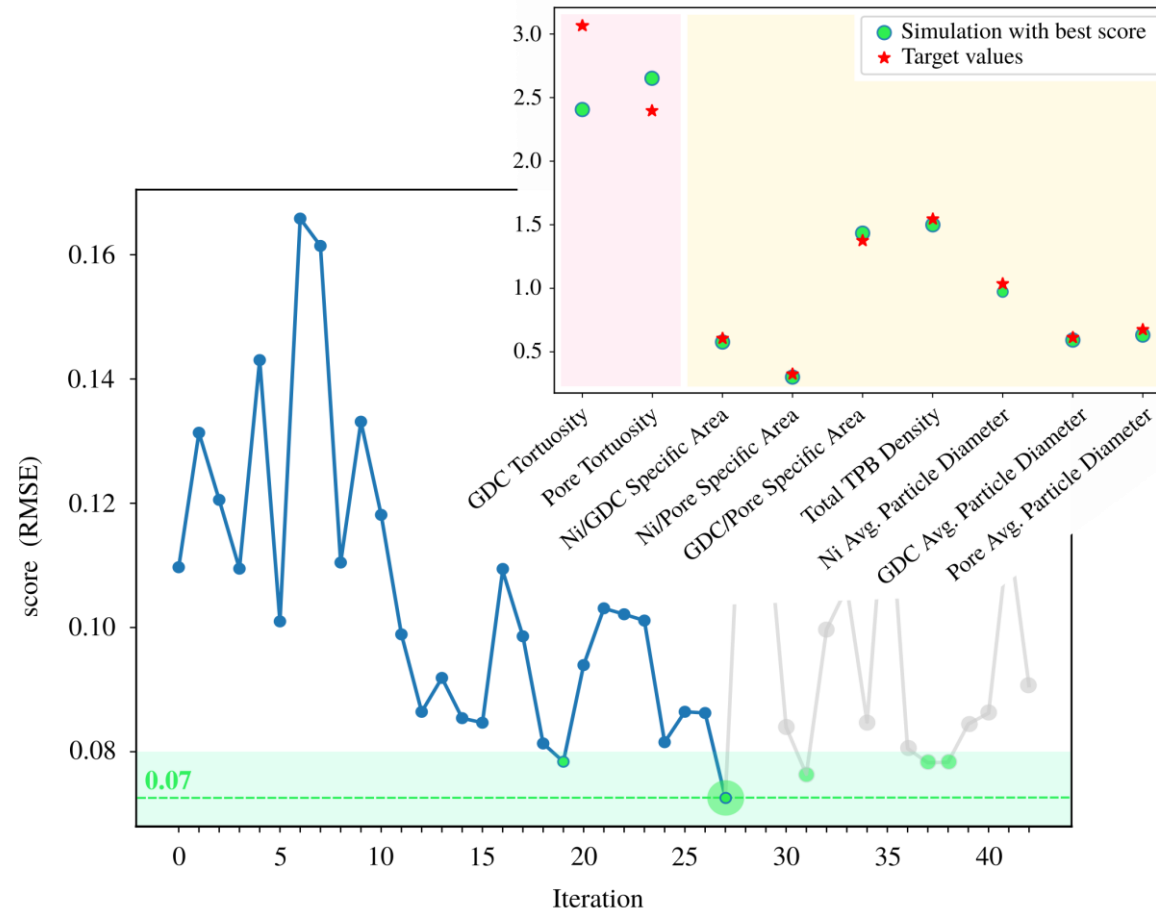
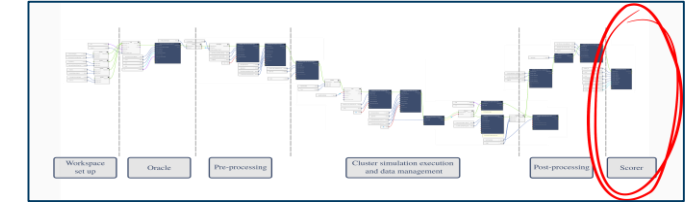
where,

$f_1(x), \dots, f_n(x) \rightarrow$ objective functions

$w_1, \dots, w_n \rightarrow$ weights

Score: RMSE of 7 meaningful microstructure parameters

GDC Tortuosity
Pore Tortuosity
Ni/GDC Specific Area
Ni/Pore Specific Area
GDC/Pore Specific Area
Total TPB Density
Ni Avg. Particle Diameter
GDC Avg. Particle Diameter.
Pore Avg. Particle Diameter.

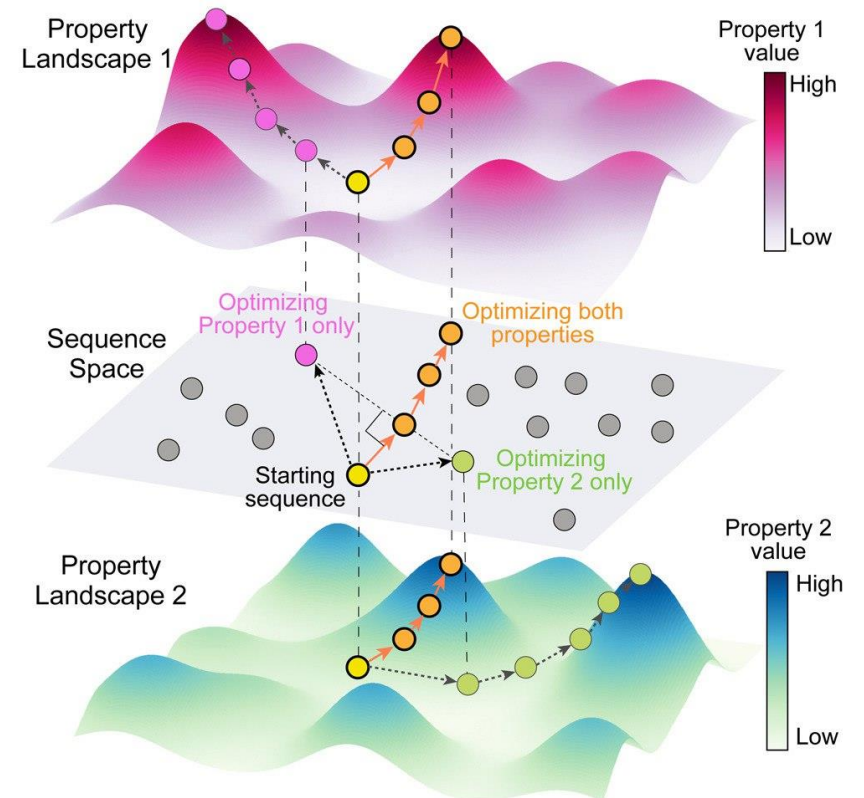
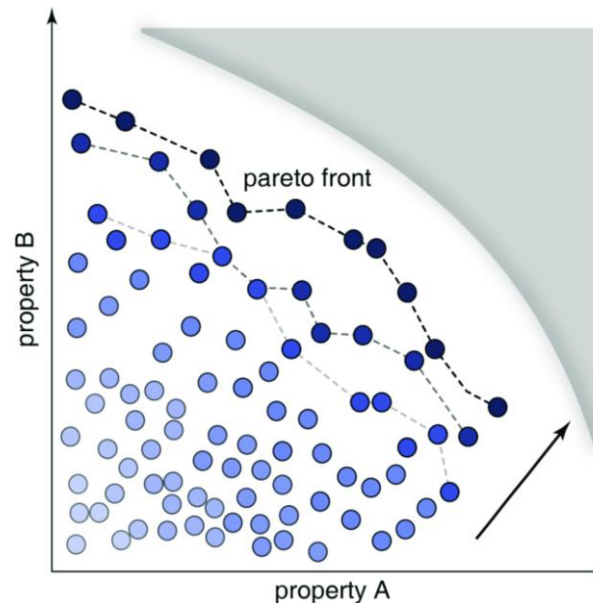


Multi-objective Optimization

- Design problems often involve more than one objective
 - Possibly conflicting objective functions

$$\begin{array}{ll}\min_{\mathbf{x}} & \{f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_n(\mathbf{x})\} \\ \text{subject to} & \mathbf{g}(\mathbf{x}) \leq 0 \\ & \mathbf{h}(\mathbf{x}) = 0\end{array}$$

- Set-valued solutions: Pareto front (objective function space), Pareto set (design variable space)
 - Search for non-dominated points
 - Best possible trade-offs between conflicting objectives

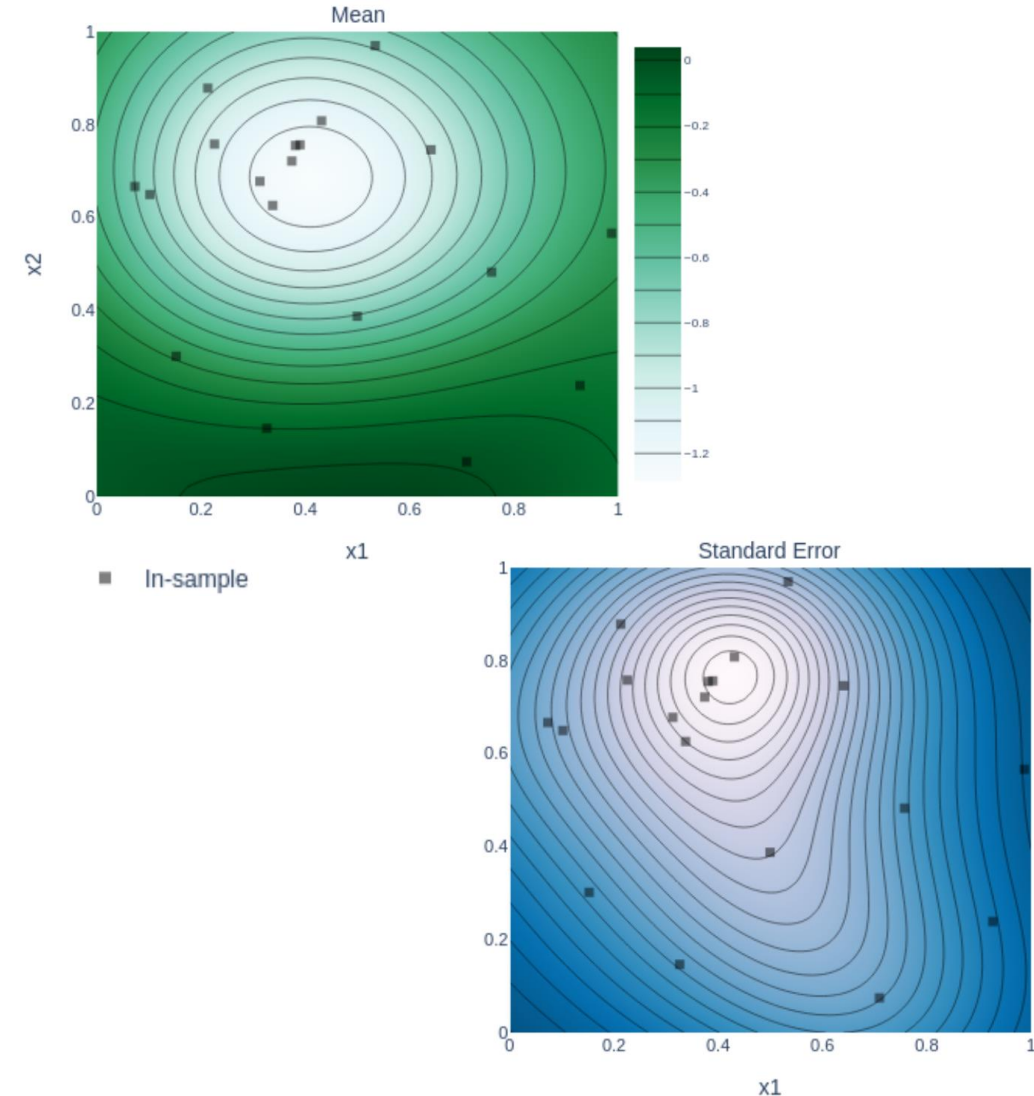


Luo, Jiaqi et al., iScience, Volume 28, Issue 3, 112119

KadiAgent

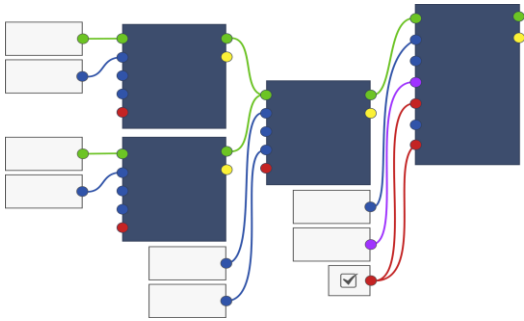
- new system

-  Ax - Adaptive Experimentation Platform
 - User-friendly wrapper for BoTorch
 - Provides higher-level APIs and infrastructure for experiment management
 - Multi-objective optimization
 - Combines built-in optimization algorithms (Sobol initialization followed by Bayesian)
 - Built-in acquisition functions (e.g., qNEHVI)
 - Visualization options (Plotly)
 - Contour plots
 - Slice plots
 - Trade-offs (plot_objective_vs_constraints)
 - Pareto frontier



KadiAgent – Trigger Options

- KadiStudio



- Kadi4Mat
 - control tags

Tags: `!kadiaagent-trial-complet...`

Tags

`!kadiaagent-umbrella-active` ✕

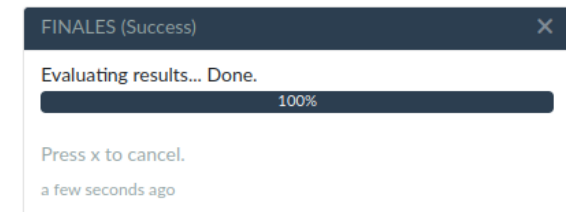
An optional list of keywords further describing the record.

`!to-finales`

`!kadiaagent-trial-running` ✕ `!to-finales`

An optional list of keywords further describing the record.

...also allow task notifications



FINALES: Human-in-the-loop automatized experiments

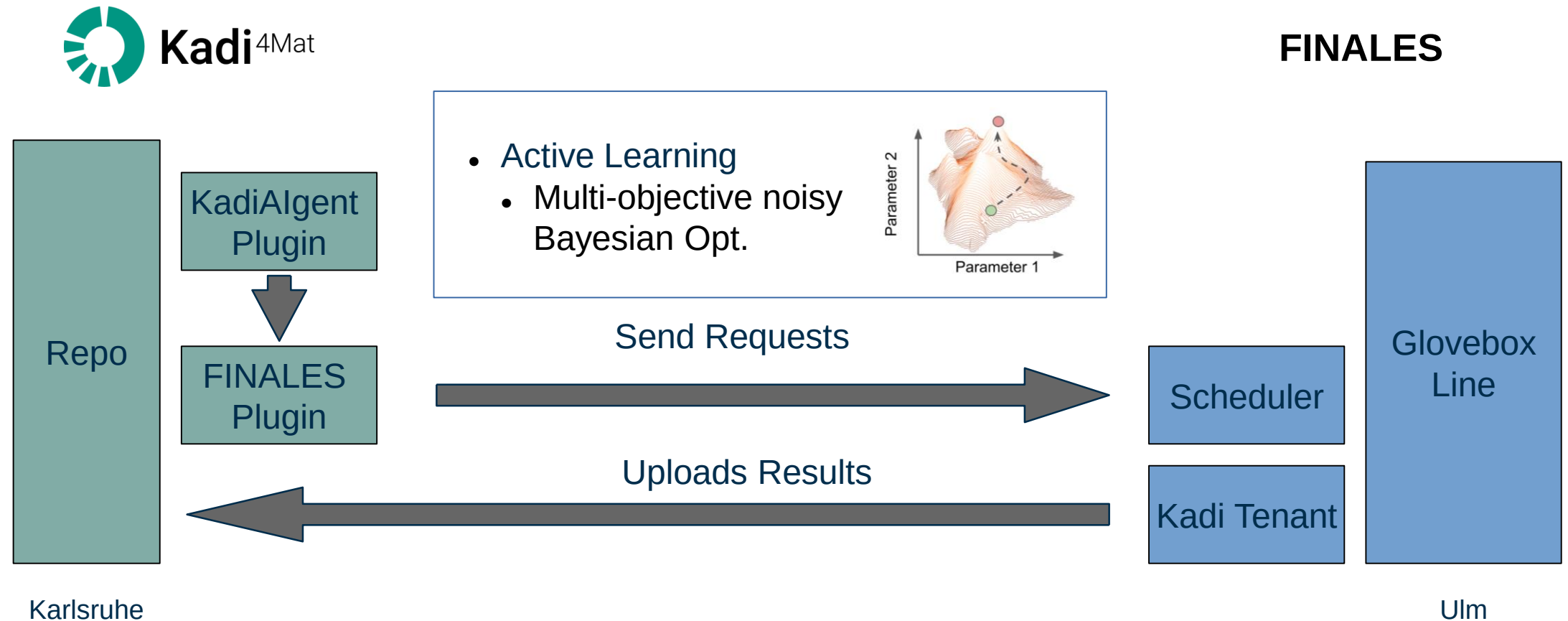
Use-case: optimizing the formation of Sodium battery systems

- Improve the efficiency of battery production vs. the lifetime of batteries
- Multi-objective optimization problem with noisy parameters and objective functions
- POLiS Cluster of Excellence: automated battery assembly glovebox in Ulm
- Project team:
 - FINALES: Monika Vogler, Leon Merker
 - Kadi4Mat: Arnd Koeppe, Giovanna Tosato, Johannes Steinhölb, Nico Brandt

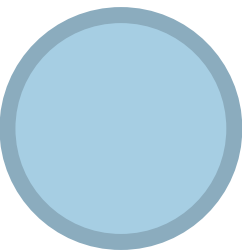


AutoBASS

Data Exchange Concept



KadiAgent: Umbrella – Trial – Interface Records



Umbrella

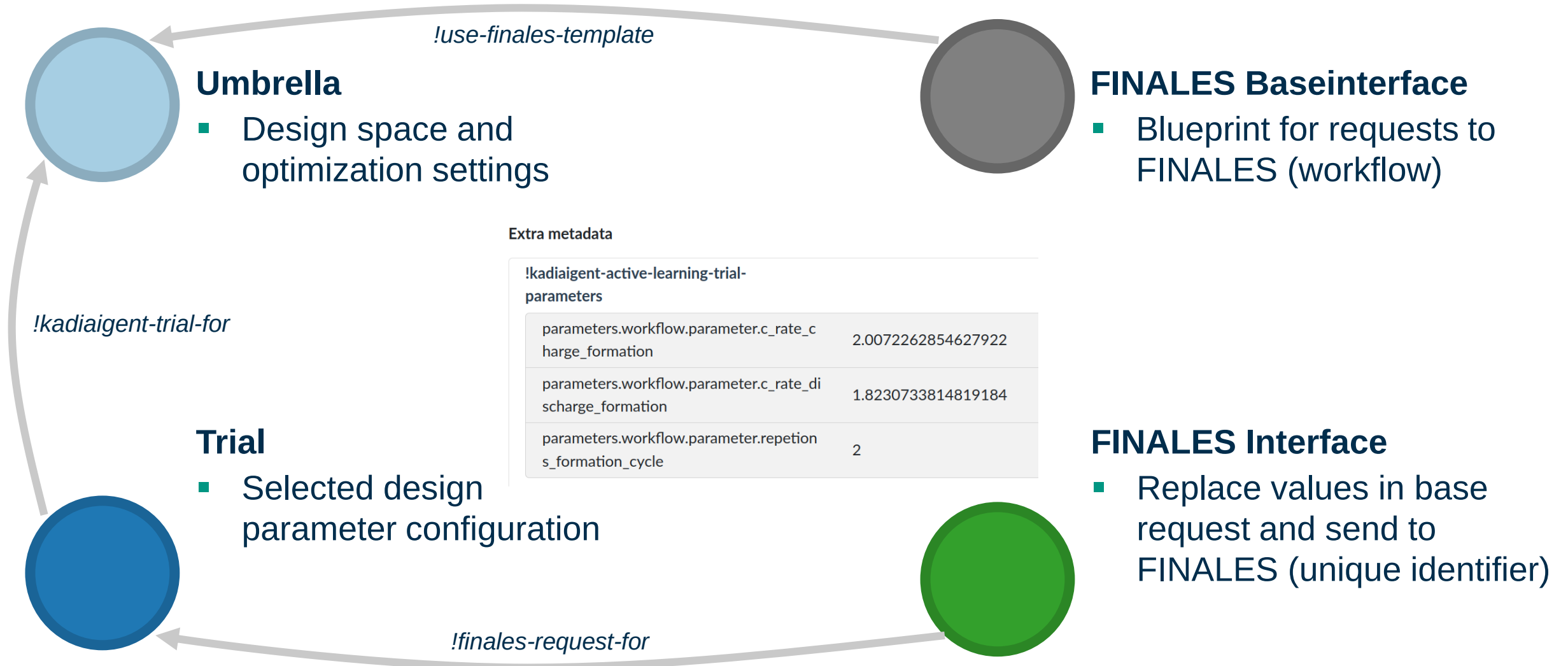
- Design space and optimization settings

Extra metadata

Show null values

!kadiaigent-active-learning-snapshot		Dictionary	
_type	AxClient	String	
experiment		Dictionary	
__type		Experiment	
search_space		Dictionary	
__type		SearchSpace	
parameters		List	
(1)		Dictionary	
__type		RangeParameter	
name	parameters.workflow.parameter.c_rate_charge_f ormation	String	
parameter_type		Dictionary	
__type		ParameterType	
name		FLOAT	
lower	0.025	Float	
upper	3	Float	

KadiAgent: Umbrella – Trial – Interface Records



KadiAgent: Evaluation

Umbrella

- Update study overview and trigger next trial

!kadiaigent-active-learning-metrics

eol_cycle_number

mean

4.75

sem

0.414578098794425

formation_time

mean

4102.135

sem

99.27835992929181

KadiAgent and FINALES plugins

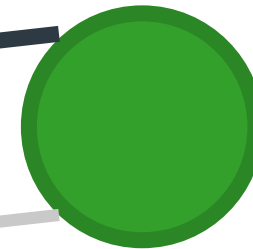
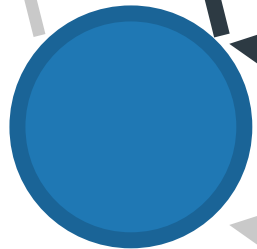
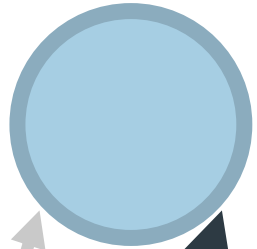
- Evaluate FINALES response and extract result metrics
- Follow links back to umbrella and update study
- Trigger next iteration

Trial

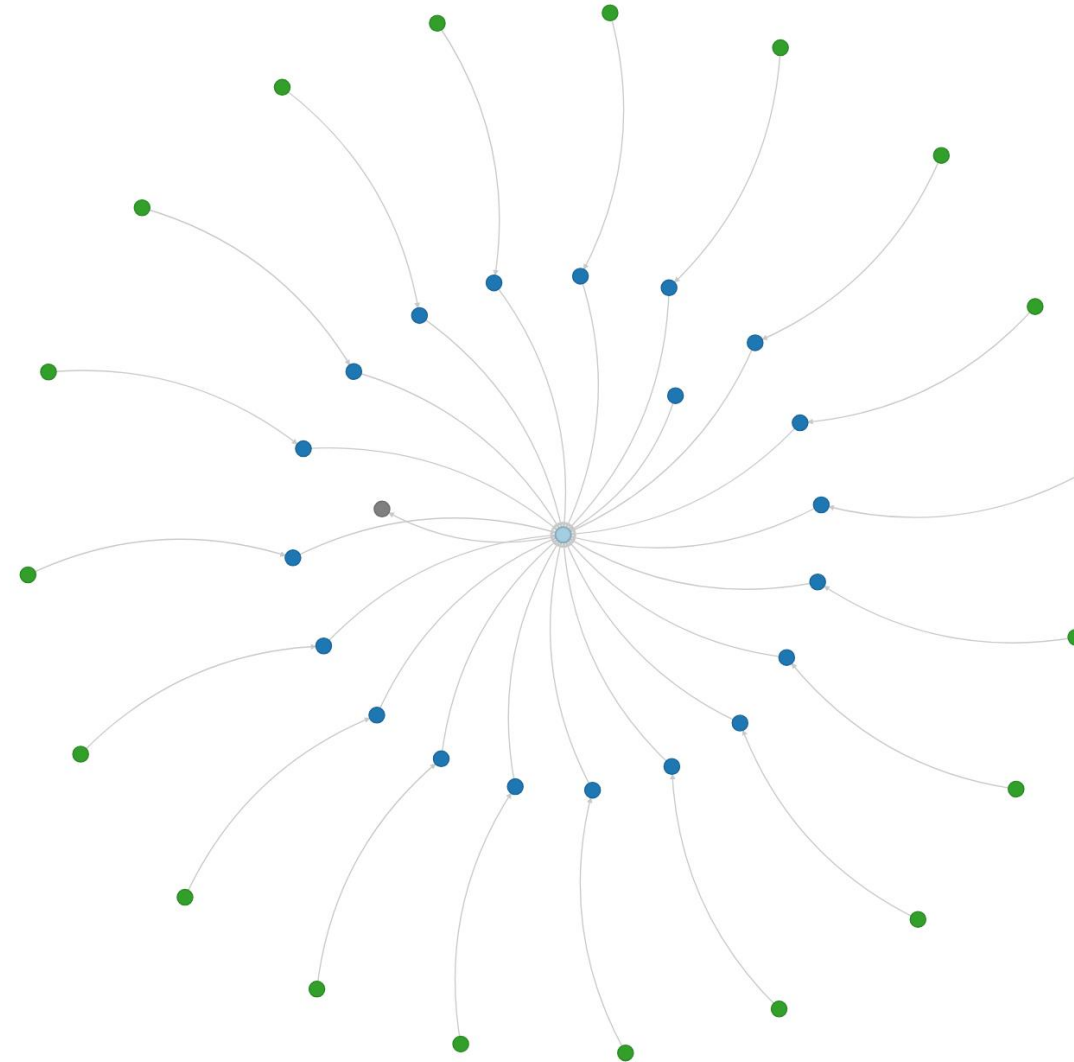
- Save result metrics

FINALES Interface

- Receives/finds response from FINALES



KadiAgent: Umbrella – Trial – Interface Records



Human interface: dashboard



Plotly figure (scatter)

- Use it as interactive figure for your project
- ▶ Here: trade-off between multiple objectives as status of study

Human interface: dashboard

Current trials				
Records 3		Sort by Last modified (newest first) ▾		
🔒 Human-Lab-AI Manual Trial 19	@human-lab-ai-manual-trial-19	Last modified 3 days ago	kadiaigent-active-le...	
🔒 Human-Lab-AI Manual Trial 18	@human-lab-ai-manual-trial-18	Last modified 3 days ago	kadiaigent-active-le...	
🔒 Human-Lab-AI Manual Trial 17	@human-lab-ai-manual-trial-17	Last modified 3 days ago	kadiaigent-active-le...	

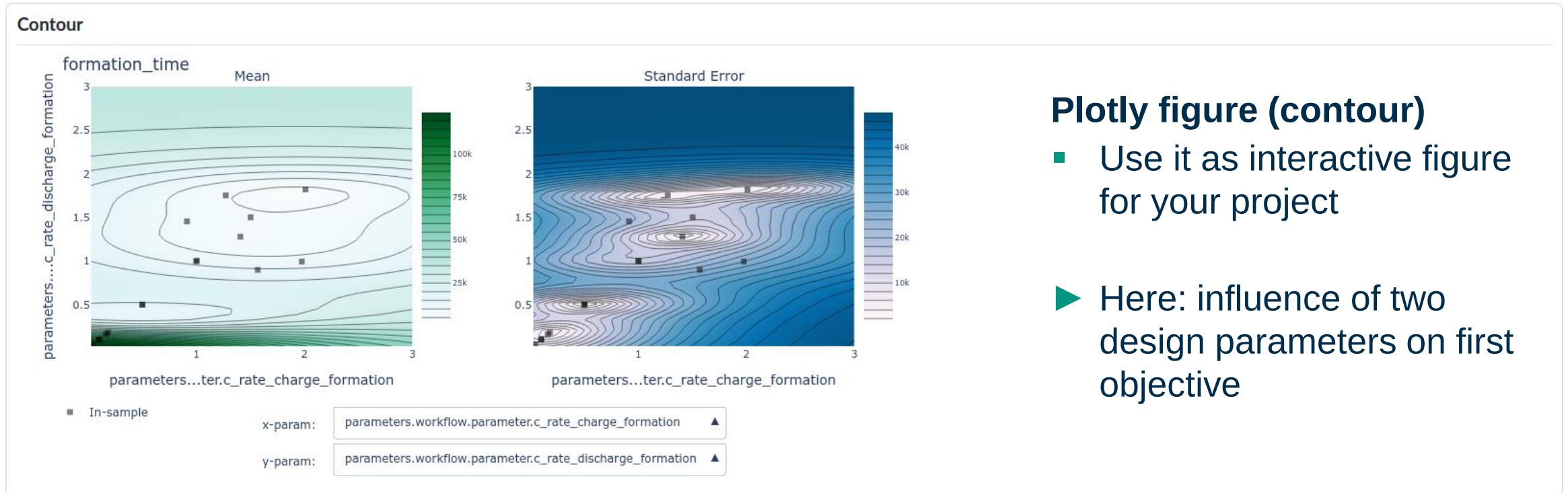
Completed trials				
Records 16		Sort by Last modified (newest first) ▾		
🔒 Human-Lab-AI Manual Trial 16	@human-lab-ai-manual-trial-16	Last modified 3 days ago	kadiaigent-active-le...	
🔒 Human-Lab-AI Manual Trial 15	@human-lab-ai-manual-trial-15	Last modified 3 days ago	kadiaigent-active-le...	
🔒 Human-Lab-AI Manual Trial 14	@human-lab-ai-manual-trial-14	Last modified 3 days ago	kadiaigent-active-le...	
🔒 Human-Lab-AI Manual Trial 13	@human-lab-ai-manual-trial-13	Last modified 11 days ago	kadiaigent-active-le...	
🔒 Human-Lab-AI Manual Trial 12	@human-lab-ai-manual-trial-12	Last modified 11 days ago	kadiaigent-active-le...	
🔒 Human-Lab-AI Manual Trial 11	@human-lab-ai-manual-trial-11	Last modified 11 days ago	kadiaigent-active-le...	

<< < Page 1 of 3 > >>

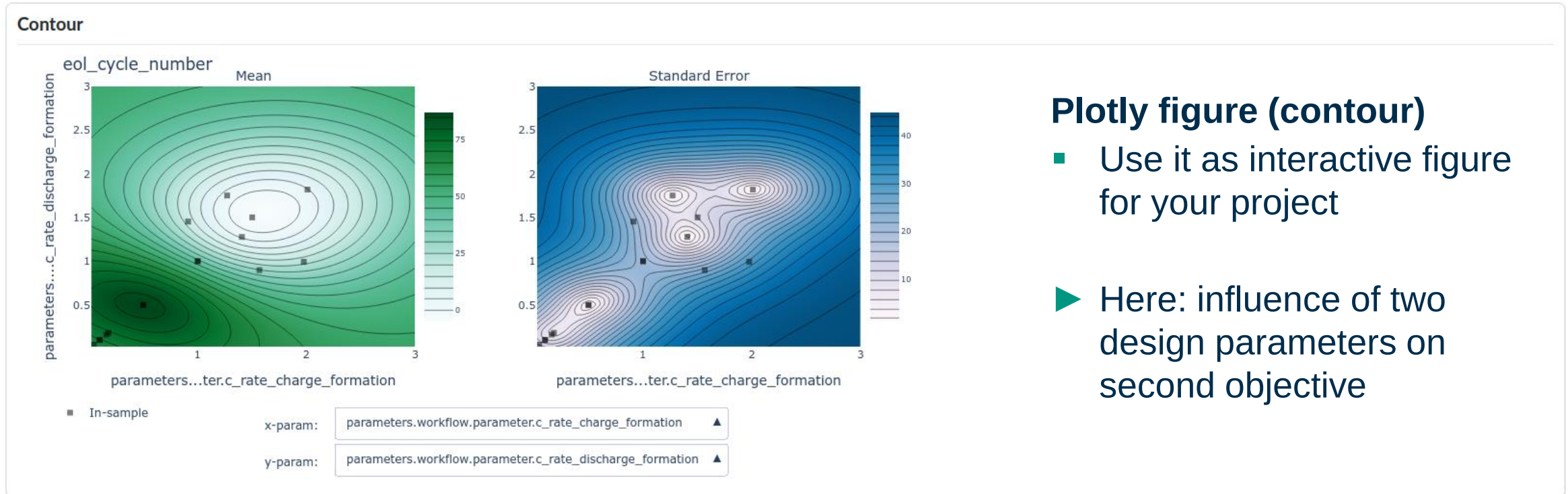
Record view

- Use it to quickly skim, access, or create specific records from your project
- ▶ Here: shows the currently running and completed trials

Human interface: dashboard



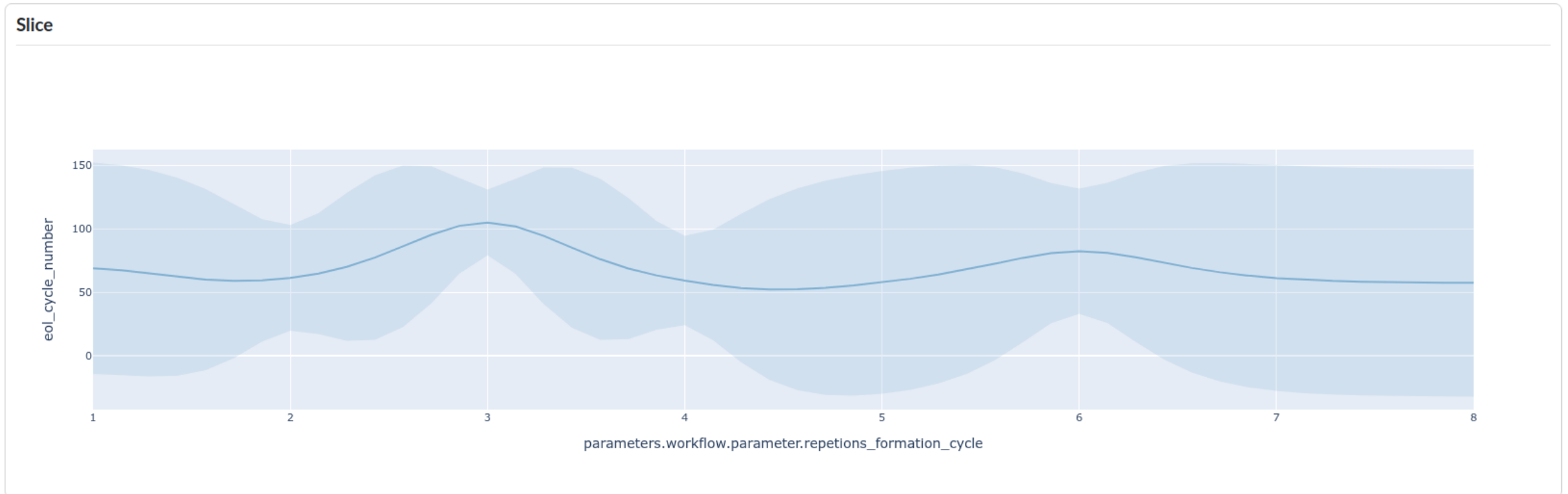
Human interface: dashboard



Plotly figure (contour)

- Use it as interactive figure for your project
- ▶ Here: influence of two design parameters on second objective

Human interface: dashboard



Plotly figure (lines)

- Use it as interactive figure for your project
- ▶ Here: model-based estimate of influence of design parameter on objective

Human interface: dashboard



Plotly figure (lines)

- Use it as interactive figure for your project
- ▶ Here: model performance and study progress

Conclusion

5

Conclusion

RDM

- Belongs to the everyday life of all researchers
- Is essential to make research data FAIR
- Promotes structured documentation and seamless provenance tracking
- Supports interoperability and reuse of data components in future workflows

Data-integrated AI

- Creates data-driven solutions for materials science
- Within KadiAI and CIDS, structures and accelerate ML research
- **KadiAgent** plugin and workflow nodes for manual and automatized experiments (multiobjective) optimization

A systematic integration of data science tools through research data infrastructure **accelerates research**

Further Information

All information about Kadi4Mat can be found under

<https://kadi.iam.kit.edu/>

Thank you for your attention!