Simulation Data Lake

FAIR aspects

CINECA

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Agenda

1. Simulation Data Lake: **brief overview**

2. Using the SDL:
   - **Web portal**
   - **Command Line Interface (CLI)**
   - **API**

3. SDL **FAIR** support

1. Simulation Data Lake: brief overview

What is the main purpose for which SDL was created?

Store large amounts of **simulation** data

Allow **access** to data in order to facilitate **reusability**

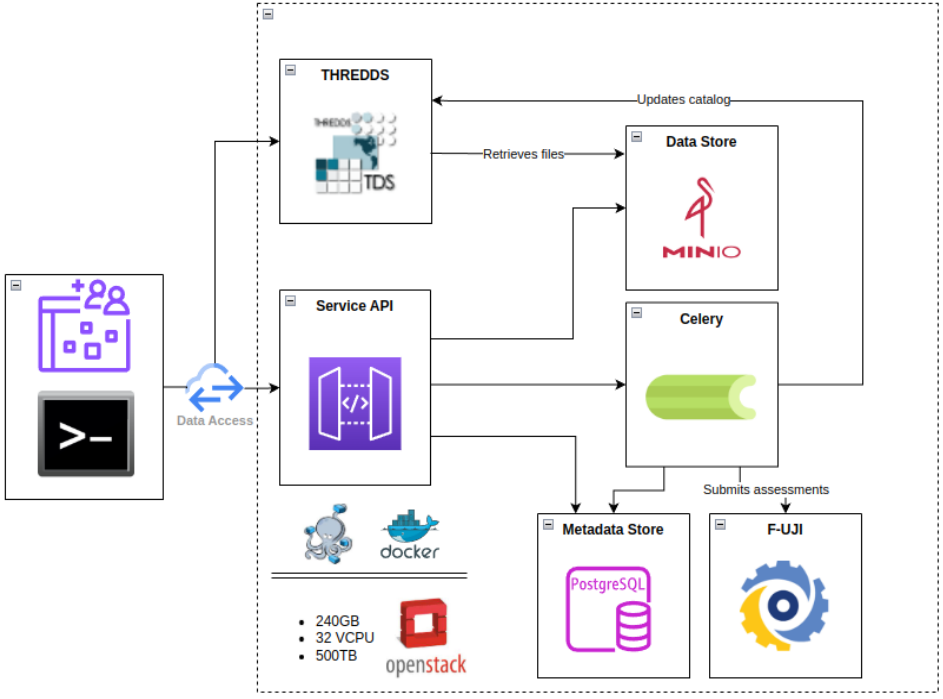
Provide **search** capabilities to find data more **efficiently**

SDL Architecture

Modular architecture and Object Storage

Hosted on **CINECA's Cloud Infrastructure**

- Restful APIs
  - Containerized services: IAM, Catalog, Async Processing
- Data Store: MinIO
  - Compatible with S3
  - Object Storage
- Metadata Store: PostgreSQL - PostGIS
  - Data model
  - Enable data search
- IaaS & Container
  - Docker, Docker-Compose
  - OpenStack

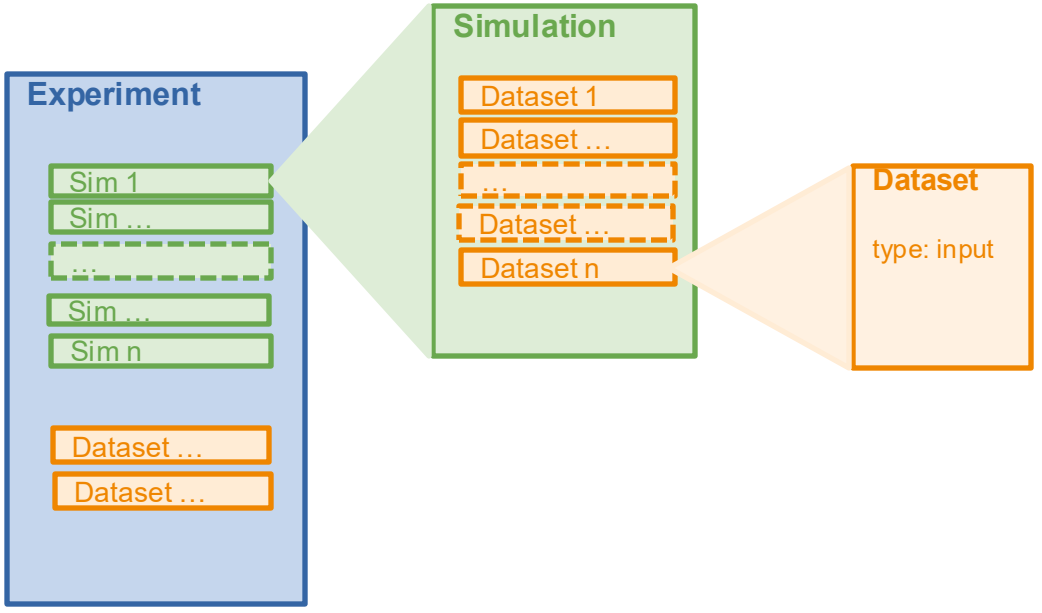


Data Model

- Main Entities:
  - Experiment
  - Simulation
  - Workflow
  - Dataset

- A Dataset can be of the following types:
  - Input
  - Output
  - Data product
  - Input parameter

- A Simulation is the execution of a Workflow and contains input data and the result of that specific workflow run.



Mapping the data/metadata to the SDL data model and v.v.

Input metadata in **json** format with **schema** described at the following link:

https://sdl-dev.hpc.cineca.it/api/bulk-import/schema?ajvStrict=true

Or using a RO-Crate metadata file

The metadata file is output in:

- JSON format
- RO-Crate format to improve fairness aspects especially interoperability

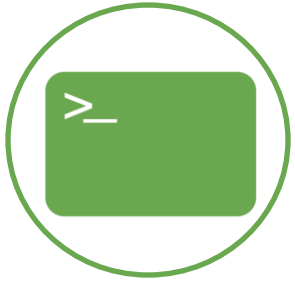
Additional functionalities

- Experiment publication: Restricted, Open access, Embargoed
- DOI minting and management
- Integration with EPOS Data Portal
- OGC Services
- Uploading and downloading both data and metadata (RO-Crate,…)
- Workflow management (CWL files and diagram visualisation)
- Dashboard of KPIs: automated FAIR assessment with **F-UJI tool**
- Data proximity and integration with CINECA HPC systems
- Advanced search functionalities including search by spatial and temporal coverage

How to access the SDL

WEB PORTAL

- User friendly interface
- Simple access to data
- For non-technical users



Command Line Interface

- For large quantities of experiments, simulations and datasets
- For technical users

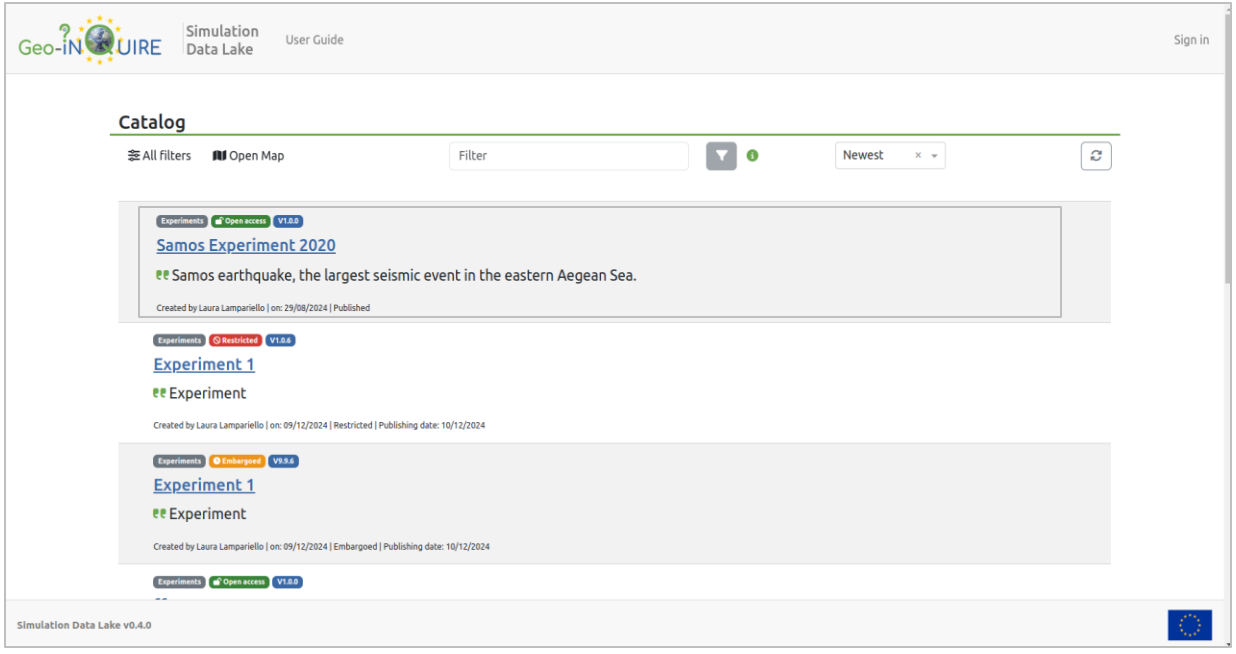
API

- Interact programmatically
- Integration with other services
- For technical users

2. Using the SDL: Web Portal

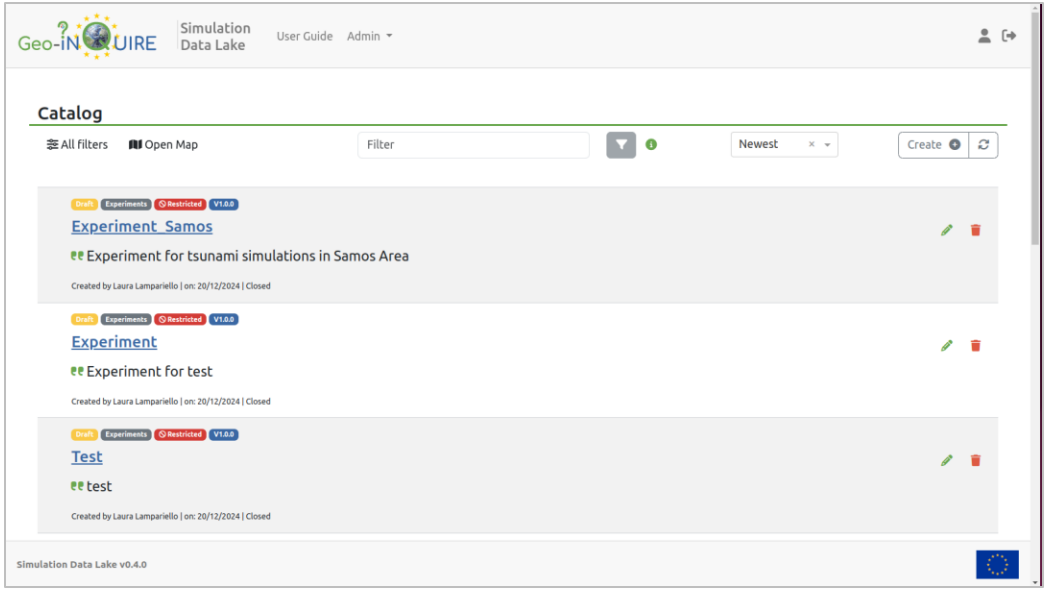
Web portal: Public Catalog

- Everyone can access
- It is possible to see the list of:
  - Experiments
  - Simulations
  - Datasets
- Only published experiments are visible
- The experiment can be published with some policies:
  - Restricted access
  - Embargoed
  - Public access
- Available only limited features



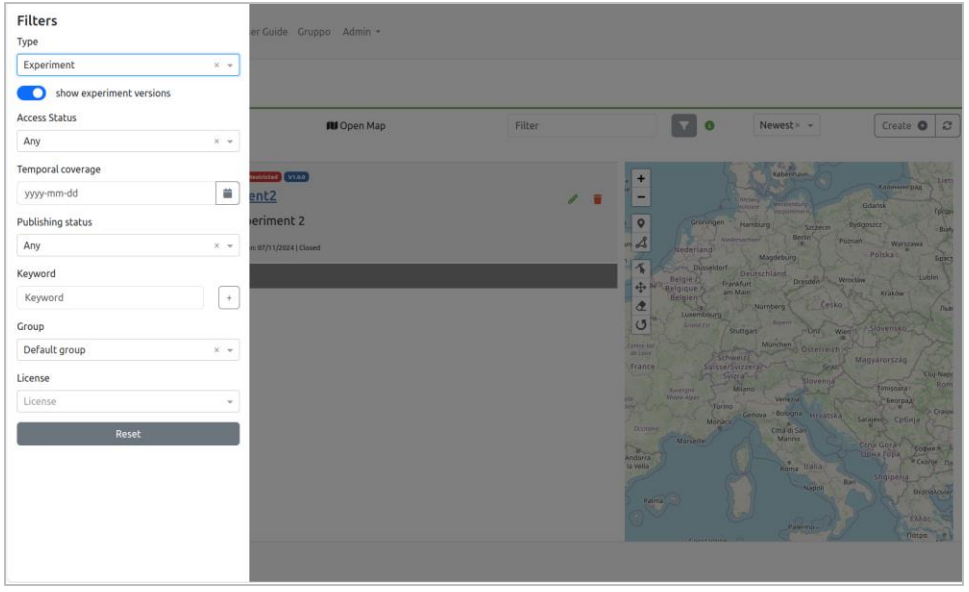
Web portal: Catalog

- Logged users can see also non published experiments
- Unpublished experiments can be seen by:
  - the creator
  - users who are part of the same group as the creator
  - the collaborators
- The catalog is paginated, the list of elements is divided over several pages

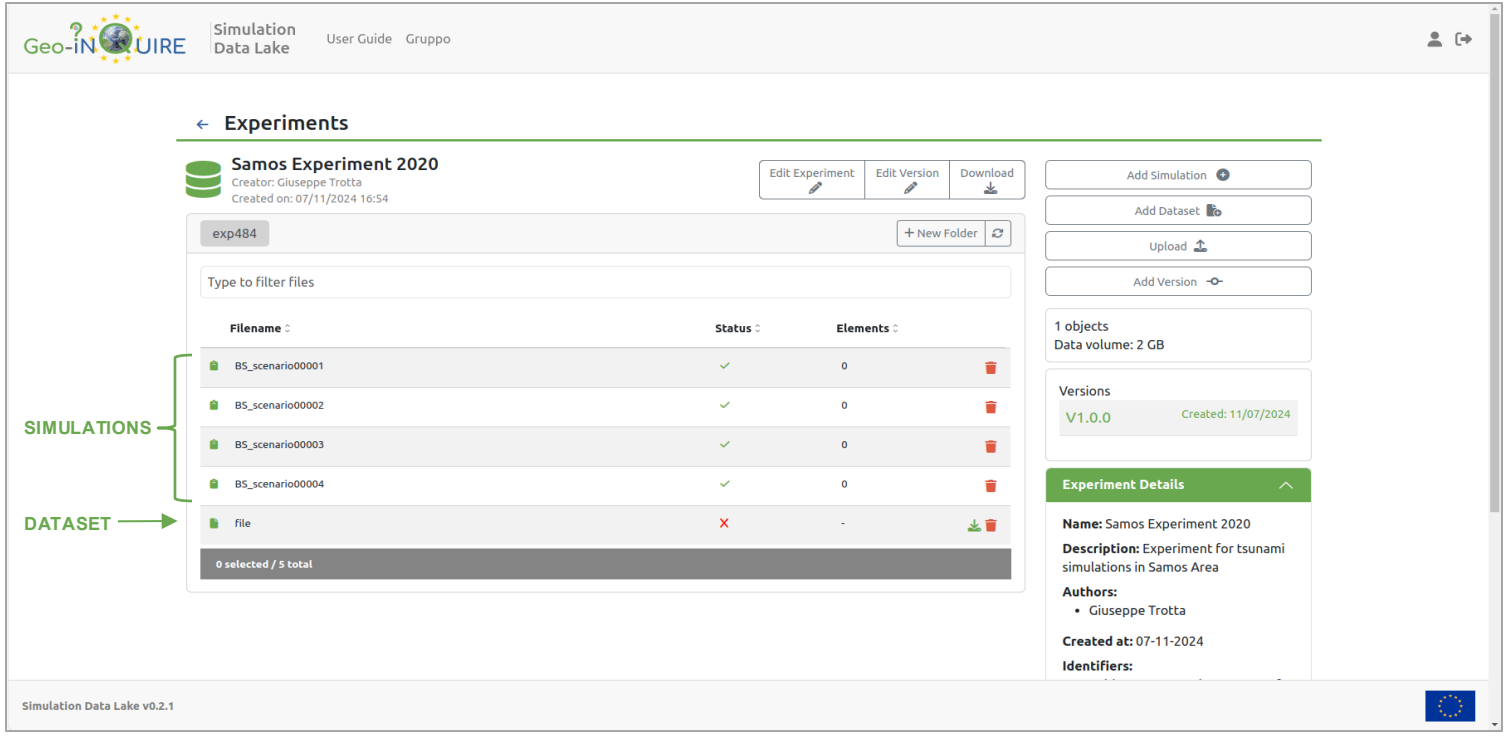


Web portal: Catalog Filters

- Filtering by **data type**: Experiment, Simulation, Dataset
- Show/hide **versions of experiments**
- Filtering by **Access Status** (Open Access, Restricted, Embargoed, Any), **Temporal coverage**, **Keywords** and **License** type
- Only logged users can search by:
  - **Publishing status** (Published, Draft, Any): whether an experiment has been published or not
  - **Group**: group with which the entity is associated



Web portal: Experiment view



2. Using the SDL: Command Line Interface

Command Line Interface (CLI): Getting started

- SDLCTL (Simulation Data Lake ConTroL)
- You can install it using two methods:
  - a remote script
  - in a virtual enviroment
- Installing the CLI you will also install a Python 3 module (SDK) to perform CLI operations from within Python code
- You can find the details of the steps to follow for installation at the following documentation link:

https://sdlctl.readthedocs.io/latest/getting_started/installation/

Command Line Interface (CLI): Commands

Look for experiments

```
(.venv) gtrotta@NGTROTTA0205932:~/Projects/geo-inquire/sdlctl$ sdlctl experiment list
                                    Experiments
```

ID	Name	Description	Created At
44	Cinzia test	Cinzia experiment for metadata ONLY: pls do NOT load any content	2024-05-03 14:16:45
30	Tsuanmi GC12	An example experiment.	2024-04-11 10:23:32
26	Lucia	Tsunami silumations	2024-04-05 14:52:31
23	Davide's Experiment	Testing upload service	2024-03-04 13:47:09
21	New CLI Experiment	This is another stupid test.	2024-02-29 18:04:03
12	Another Experiment	A test experiment after some refactoring.	2024-02-28 09:48:47
11	My second CLI experiment	This is another experiment created with the CLI in a more fancy way.	2024-02-27 18:10:41
9	My Experiment	Just a simple test.	2024-02-27 13:19:41
7	test	My first test experiment	2024-02-01 22:14:37

```
                                    Press 'q' di quit.
```

Delete confirmation

```
 % sdlctl file upload                                          ~ NMPUCCINI205808
Experiment ID: 12
Filename: sample50M
  Calculating MD5... ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 100% 0:00:00

Starting new upload of file: sample50M

  Calculating MD5... ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 100% 0:00:00
  Uploading...       ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 100% 0:00:00

Upload completed successfully!

 % sdlctl file delete                                          ~ NMPUCCINI205808
Experiment ID: 12
Filename: sample50M
Are you sure you want to delete the file? [y/N]:
```

Upload resume

```
 % sdlctl file upload -id 12 -f sample50M                      ~ NMPUCCINI205808
  Calculating MD5... ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 100% 0:00:00

Starting new upload of file: sample50M

  Calculating MD5... ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 100% 0:00:00
  Uploading...       ╸━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━  30% 0:00:05^C
Upload interrupted by user.
  Calculating MD5... ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 100% 0:00:00
  Uploading...       ╸━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━  40% 0:00:04
 % sdlctl file upload -id 12 -f sample50M                      ~ NMPUCCINI205808
  Calculating MD5... ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 100% 0:00:00

Resuming upload of file: sample50M

  Calculating MD5... ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 100% 0:00:00
  Uploading...       ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 100% 0:00:00

Upload completed successfully!

 %                                                             ~ NMPUCCINI205808
```

See the following documentation for the complete list of commands: https://sdlctl.readthedocs.io/latest/reference/commands/

Wizard

- Help researchers generate the metadata file
- Through a guided procedure, it automatically generate an experiment metadata JSON file by analysing the structure of an input folder.
- It maps folder hierarchy to metadata, detects patterns in files and folders to minimize repetitive input, and guides users through the classification process.
- It is intended to be used with high item count for better results.
- Beta version
- Documentation:
  - https://sdlctl.readthedocs.io/latest/getting_started/wizard/
  - https://sdlctl.readthedocs.io/latest/tutorials/5-wizard/

3. Using the SDL: API

API specs

OpenAPI Specification
https://sdl.hpc.cineca.it/api/docs

upload

- POST `/api/experiments/{experiment_id}/init-upload/{filename}` init upload of a file
- POST `/api/experiments/{experiment_id}/upload` upload file
- POST `/api/experiments/{experiment_id}/complete-upload/{upload_id}/{key}` complete upload

download

- POST `/api/experiments/{experiment_id}/download/{filename}` download a file
- GET `/api/experiments/{experiment_id}/init-download/{filename}` Initialize download of a file

experiment

- POST `/api/experiments` Create a new experiment
- GET `/api/experiments` Get experiments
- GET `/api/experiments/{experiment_id}` Get an experiment by id
- DELETE `/api/experiments/{experiment_id}` Delete an experiment
- PATCH `/api/experiments/{experiment_id}` Update experiment data
- DELETE `/api/experiments/{experiment_id}/files` Delete files whose name begin with a certain prefix in a given experiment (if path ends with '/' it will look for a directory to delete, otherwise, a file)
- GET `/api/experiments/{experiment_id}/files` Get list of files for an experiment
- POST `/api/experiments/{experiment_id}/collaborators` Add a collaborator to the experiment

simulation

- GET `/api/experiments/{experiment_id}/simulations` Get all simulations of an experiment
- POST `/api/experiments/{experiment_id}/simulations` Create a new simulation
- PATCH `/api/experiments/{experiment_id}/simulations` Modify a new simulation
- POST `/api/experiments/{experiment_id}/simulations/{folder_name}` create a simulation folder or a simple folder

3. SDL FAIR support

Improving FAIRness in the SDL

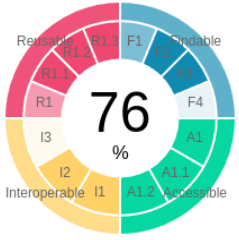
- Automated periodic FAIR assessment
  - Ensures continuous monitoring and improvement
  - F-UJI tool used to assess experiments FAIRness

- Incremental improvements:
  - Agile, step-by-step enhancements to FAIR compliance

SDL FAIR details

- The first FAIR assessments using FUJI gave us a 5% score

- The result of a FAIR assessment performed recently on an SDL experiment:



	Score earned:	Fair level:
Findable:	4 of 7	moderate
Accessible:	7 of 7	advanced
Interoperable:	4 of 6	moderate
Reusable:	5 of 6	moderate

SDL FAIR details / Findable

- Unique identifiers:
  - UUID
- Persistent identifiers:
  - DOI (minting will be available soon)
- Metadata contains descriptive data to support findability:
  - creator, title, data identifier, publisher, publication date, summary, keywords...
- EPOS Data Portal integration

SDL FAIR details / Accessible

- Data access levels specified in metadata
- Metadata and data are retrievable by their identifier
- Standardized communication protocol used to access data and metadata

SDL FAIR details / Interoperable

- Metadata is represented using a formal knowledge representation language
  - RO-Crate

Why RO-Crate?

- Lightweight, machine-readable metadata format
- Facilitates interoperability and reusability
- Widely adopted in research data management
- Allows for CWL workflows representations using profiles such as Workflow RO-Crate

SDL FAIR details / Reusable

- Metadata specifies the content of the data
- Metadata includes license information under which data can be reused
- Metadata includes provenance information about data creation or generation

SDL FAIR details / User perspective

Findable:

- Searchable metadata catalog: Users can easily discover datasets using keywords, text search, or other filters.
- SDL catalog explorable using:
  - Web application
  - CLI
  - Python module
  - REST API
  - EPOS Data Platform (coming soon)
- DOI assignment (coming soon): Enables citation and persistent access to datasets.

SDL FAIR details / User perspective

Accessible:

- Clear access policies
- Standardized resource download mechanism: makes it easy to retrieve data programmatically or manually

SDL FAIR details / User perspective

Interoperable:

- Standard/well known formats: users can work with data using familiar tools
- RO-Crate packaging: ensures metadata and data are bundled in a machine-readable, structured way

SDL FAIR details / User perspective

Reusable:

- Rich metadata: users understand the context, origin, and structure of the data
- Clear licensing: users know how they can use the data

Useful information

- Dev: https://sdl-dev.hpc.cineca.it
  - Development environment with 1T of storage
  - It is the most updated enviroment with features in development
- Prod: https://sdl.hpc.cineca.it
  - Production environment with 500T of storage
- Contacts: sdl@cineca.it

- Request an SDL account using the following link:
  https://sdl-userguide.readthedocs.io/tutorials/Introduction/
- Documentation
  - Web Portal: https://sdl.hpc.cineca.it/docs
  - Command Line Interface: https://sdl.hpc.cineca.it/cli/docs

Thank you for your attention

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