Geo-Inquire Simulation Data lake

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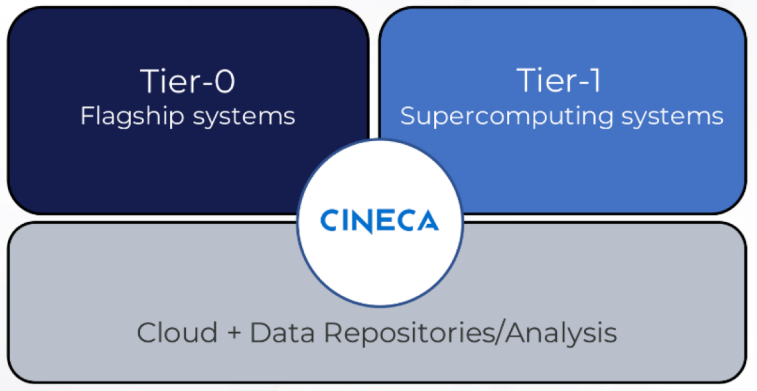
50 YEARS OF SUPERCOMPUTERS

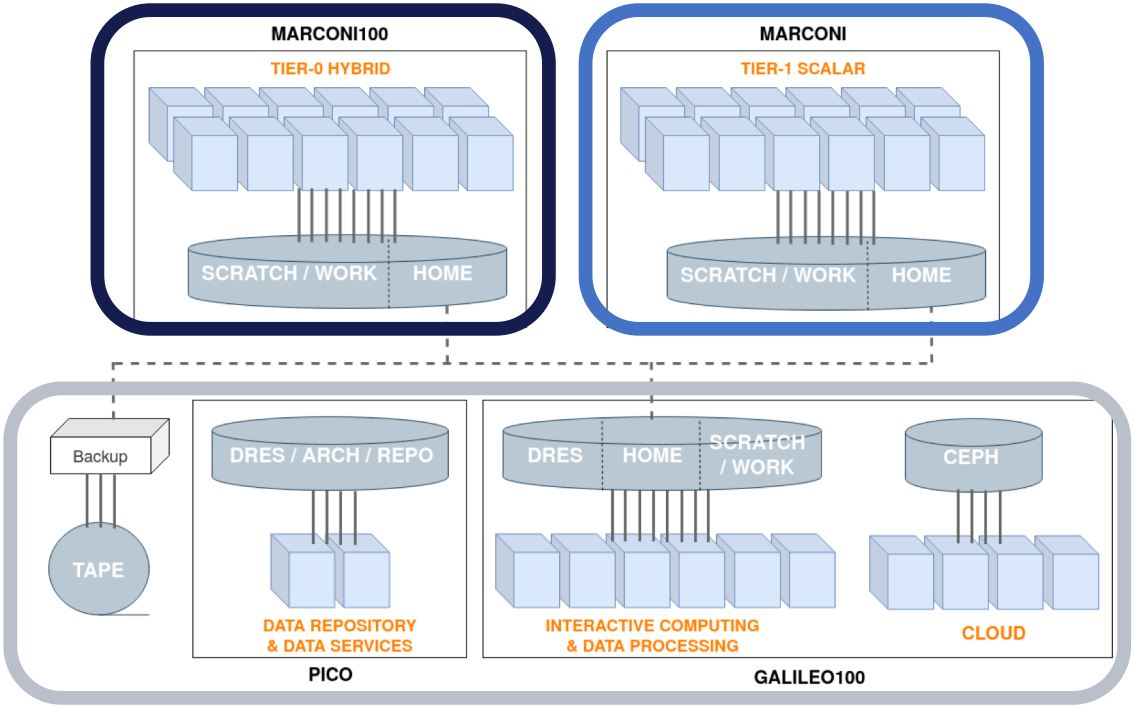
TIMELINE OF CINECA'S SUPERCOMPUTERS

1969	1975	1985	1989	1993	1994	1995	1996	1998	1999
CDC 6600	CDC 7600	CRAY X-MP / 48	CRAY Y-MP / 48 IBM 3090-600 VF	CRAY C-90/2128	CRAY T30 64	CRAY T3D 128	CRAY T3D 128	CRAY T3E 256 SGI ORIGIN 16	CRAY T3E 256 SGI ORIGIN 64 IBM SP POWER 3
	1° SC IN ITALY	1° VECTOR SC			1° PARALLEL SYSTEM		1° MPP SYSTEM		
	1 TERAFLOP/S			10 TERAFLOP/S	100 TERAFLOP/S	2 PETAFLOP/S			PRE-EXASCALE

2000	2002	2004	2005	2007	2009	2012	2016	2020	2022
VIRTUAL THEATRE	IBM SP4 612	IBM SP5 512	IBM CLX XEON 1024	IBM BCX AMD 5120	IBM SP6	FERMI	MARCONI	MARCONI100	LEONARDO

CINECA HPC INFRASTRUCTURE





2022 OVERVIEW

HPC SYSTEMS

CINECA

CINECA enables world-class scientific research by operating and supporting leading-edge supercomputing technologies and by managing a state-of-the-art and effective environment for the different scientific communities.

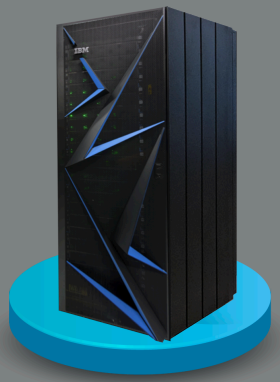
LEONARDO | 2022

4992 nodes
Booster Module:
  32 core per node
  4 GPU NVidia Ampere custom
Data Centric Module:
  56 cores per node
110 PB Storage
250 PFlops

SOON IN PRODUCTION

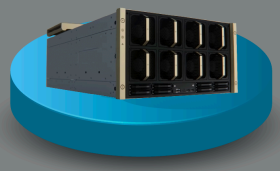
MARCONI | 2016

3188 nodes
48 cores per node
612 TB RAM
10 PFlops



MARCONI100 | 2020

980 nodes
32 cores per node
4 GPU Nvidia V100 per node
8 PB Storage
32 PFlops



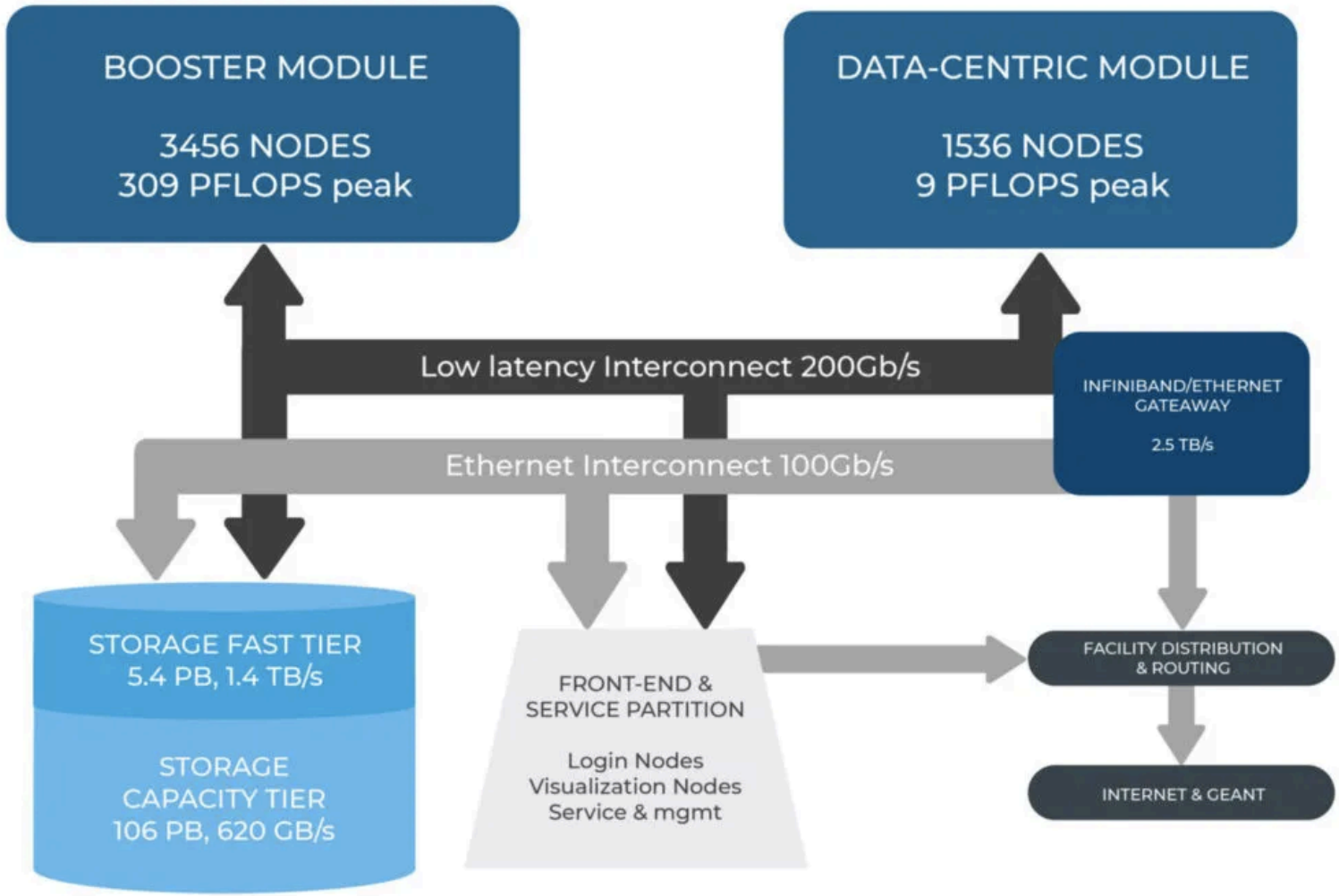
DGX | 2021

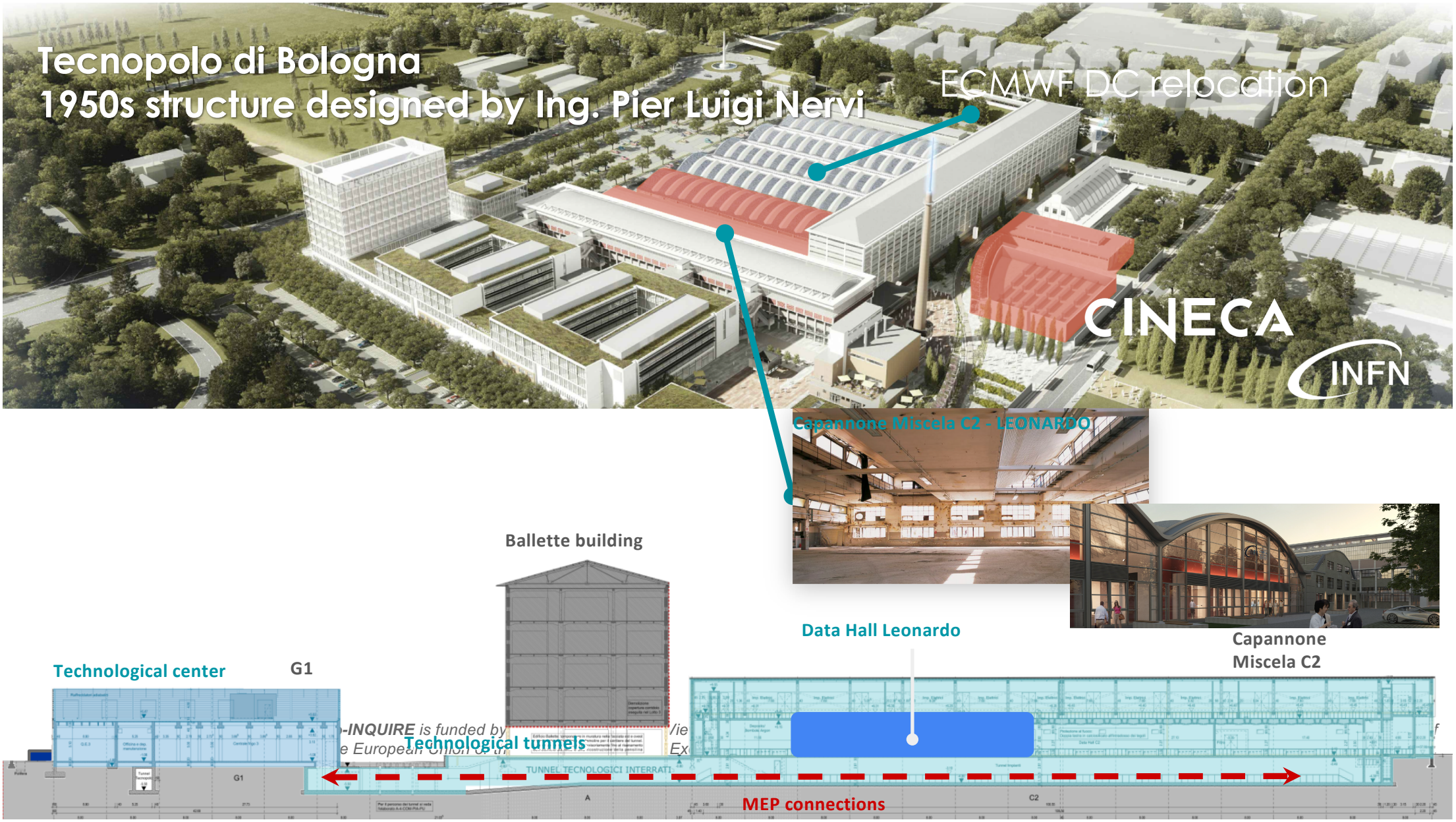
3 nodes
128 cores per node
8 GPU NVIDIA A100 per node
100 TB Storage
15 PFlops

GALILEO100 | 2021

564 nodes
48 cores per node
2 GPU NVIDIA V100 per node
~22 PB Storage
2 PFlops

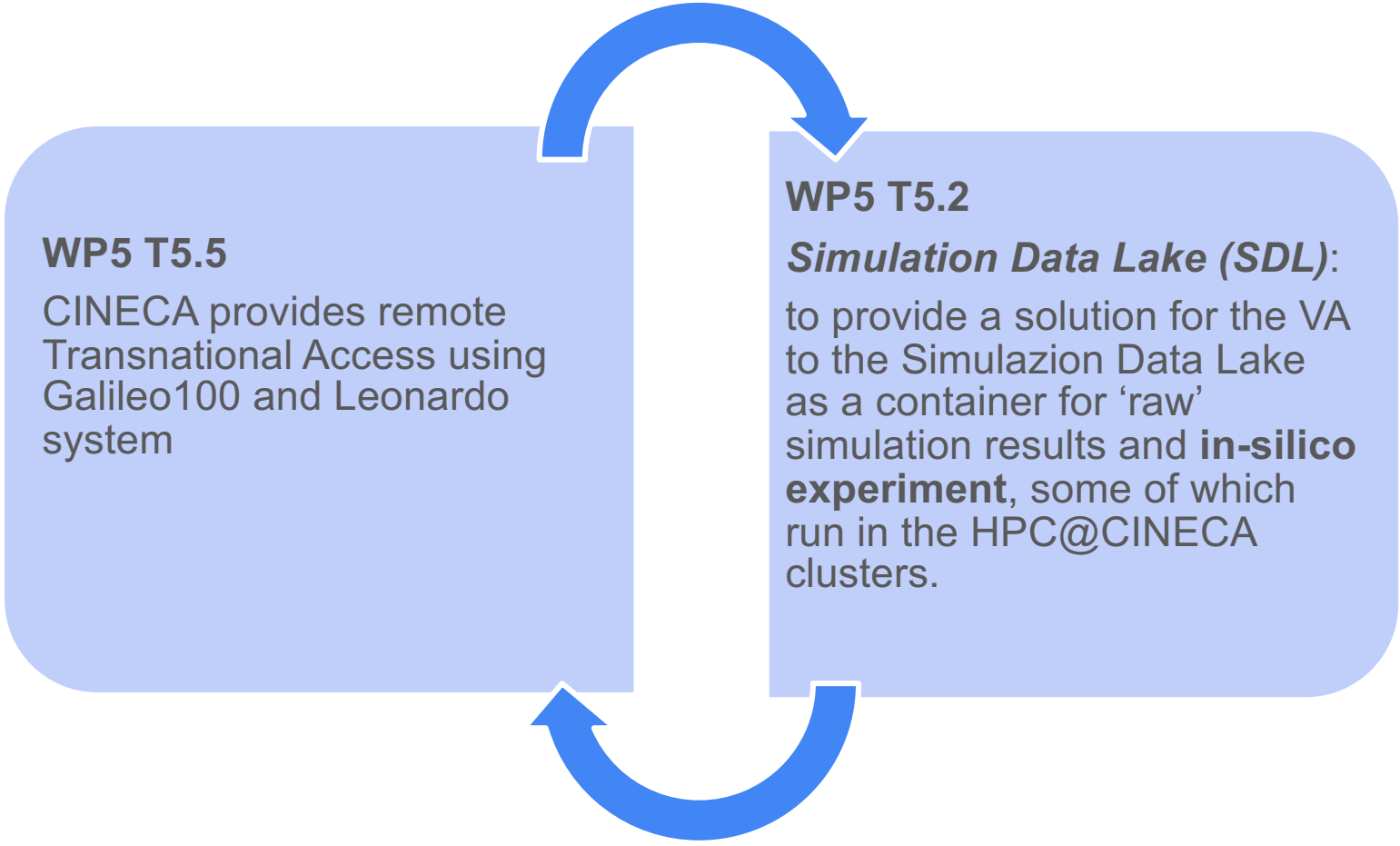
Leonardo Modular Computing





-INQUIRE is funded by

CINECA for Geo-INQUIRE



Geo-Inquire Partners requirements for the Simulation Data Lake

User Stories Questionnaire and survey:

- to better understand datasets (e.g., metadata, formats)
- to better understand the expected functionalities

USERS

- Researcher
- Developer, responsible for software in a scientific community
- Responsible for TA service (providing access to software and computational resources)
- Designer of service provider for data processing

DATA TYPE

- Inputs and outputs of simulations
- Post-processing of simulations
- Intermediate step of a WaaS
- Results of numerical benchmarks and verification tests (published previous works)

Partners requirement: experiment **reproducibility**

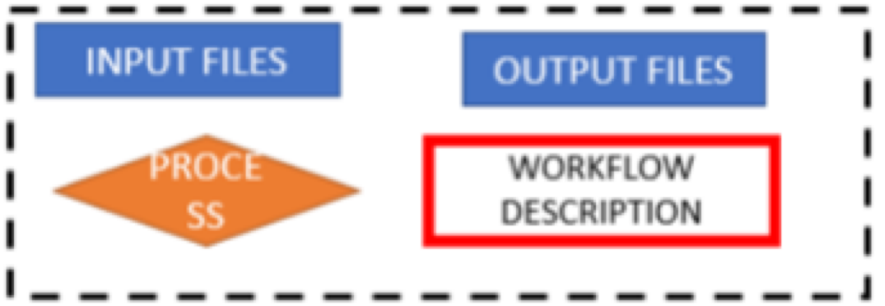
- **Dataset definition:** **Dataset ~ Experiment** (including 1-to-many simulation runs).
- **Data formats**: numerous. We need a standard, at least for outputs (e.g., netCDF, HDF5).

To have experiments reproducibility both

input (e.g., parameter files, config files, input data) and

output of simulations

must be stored in the SDL.



Additionally, the dataset could potentially include scripts/pipelines and a description of the workflow.

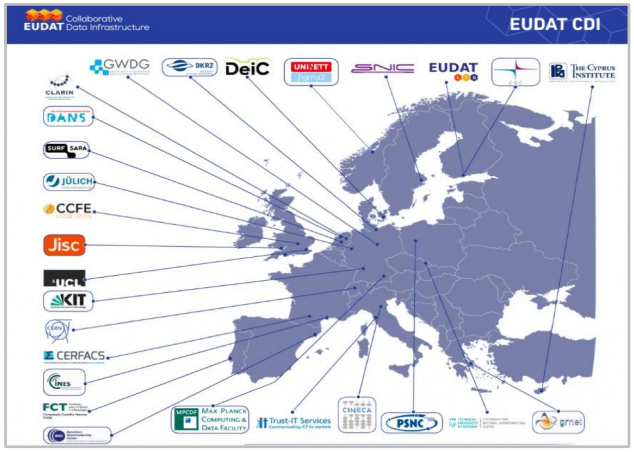
So, **a dataset should store all the data of an experiment**.

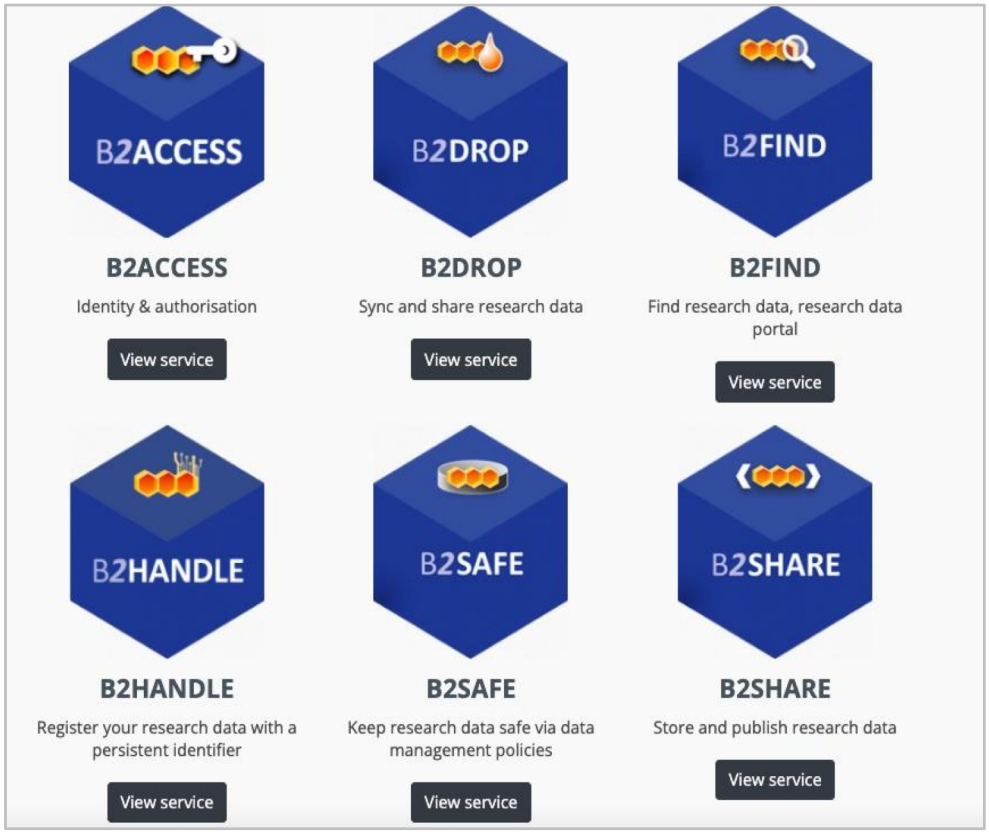
Partners requirements for the Simulation Data Lake

Use case/Functionality	Description
AAAI Authentication, Authorization, Accounting, Infrastructure	AA & tracking the access of users and the functions/functionalities they make use of
Data access policy	Define user custom data access policies: public, private, embargo
Create dataset (up to ~1TB)	Create a data collection
Add new data (single file up to ~ 1GB) to dataset	Add data to a data (files) collection
Assign a DOI	Create and assign a DOI to a data collection or object
Assign a PID	Create and assign a DOI to a data collection or object
Assign metadata (add single item and scheme)	Assign metadate. Schemes are TBD by the communities
Query data by metadata	List data matching some metadata criteria
View list of all data owned by a user	List data with a certain author
View list of all data (general usage)	List all data collections stored
View details of a specific data	View details/metadata summary
Get dataset (up to ~1TB)	Download data collection
Get individual data (single file up to ~ 1GB) from dataset	Download data object
Get data from file	Extract data from single file (temporal, geographical slice)
API exposure	API exposure for integration in post-processing pipelines

What is EUDAT?

The **EUDAT Collaborative Data Infrastructure** (or EUDAT CDI) is one of the largest infrastructures of integrated data services and resources supporting research in Europe. It is sustained by a network of more than 20 European research organisations, data and computing centres.

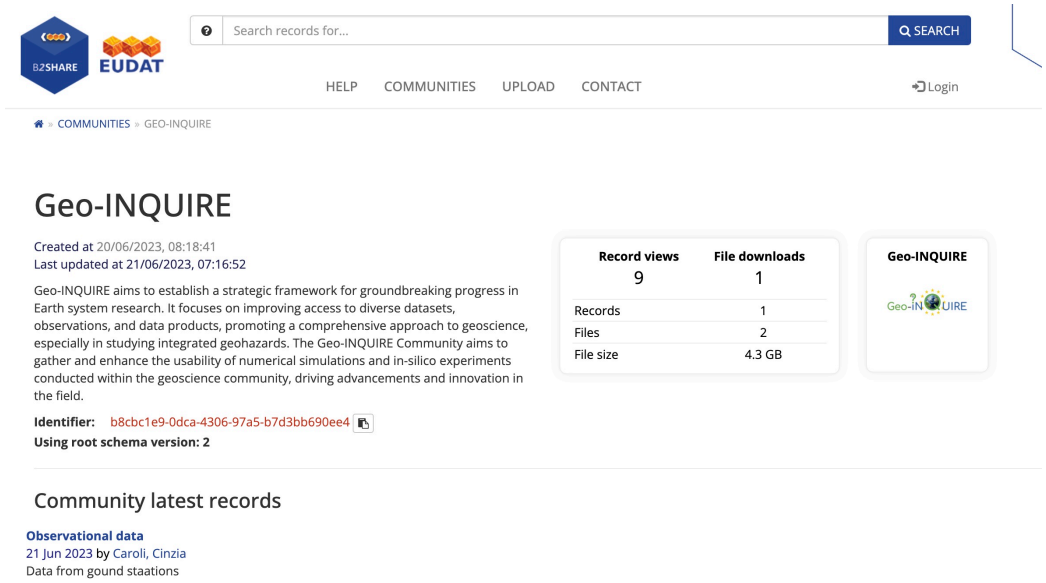




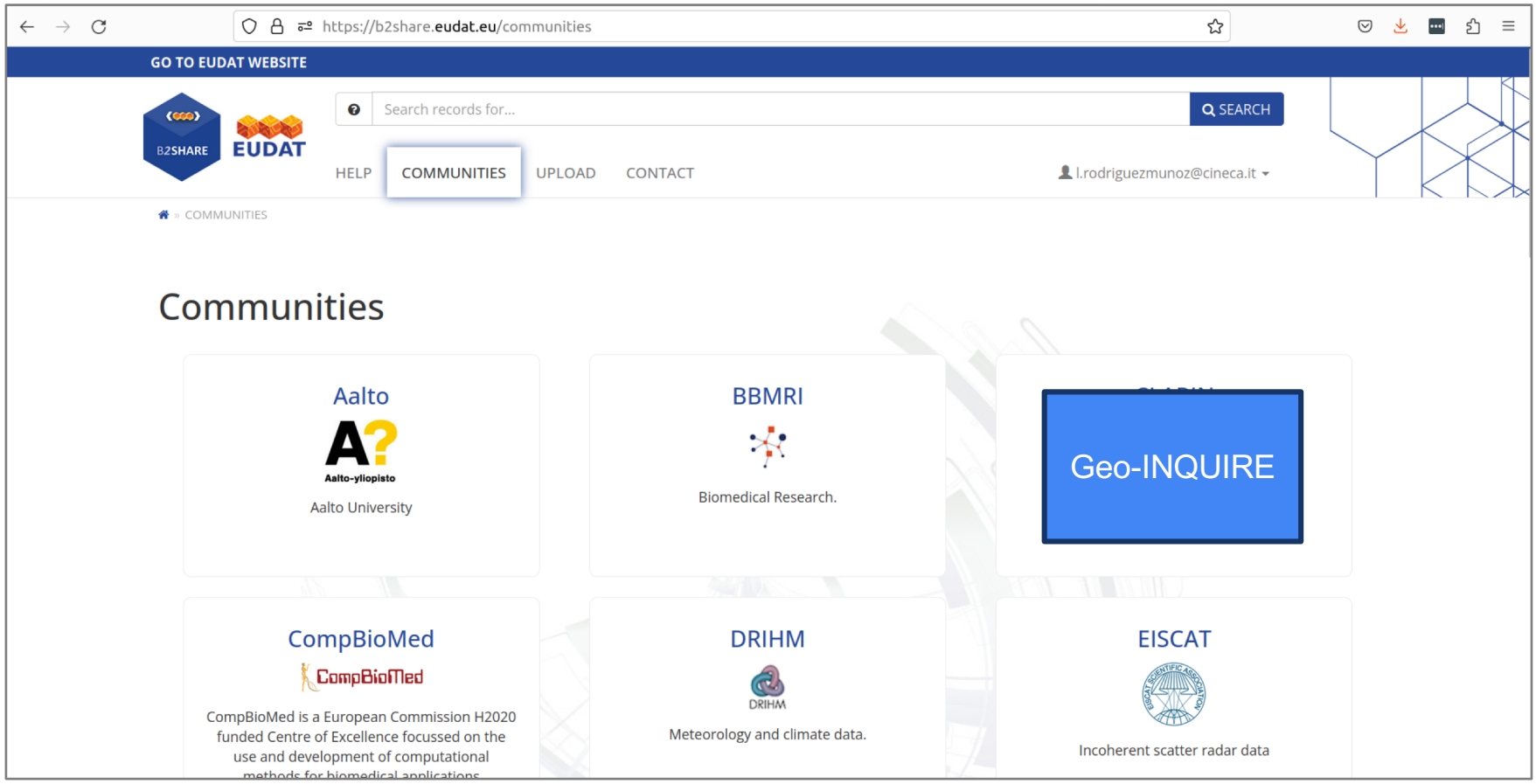
Geo-Inquire SDL solution based on B2SHARE

- storing and publishing scientific data
- Find dataset through Metadata
- Assign PID and DOI
- API exposure and Web-platform

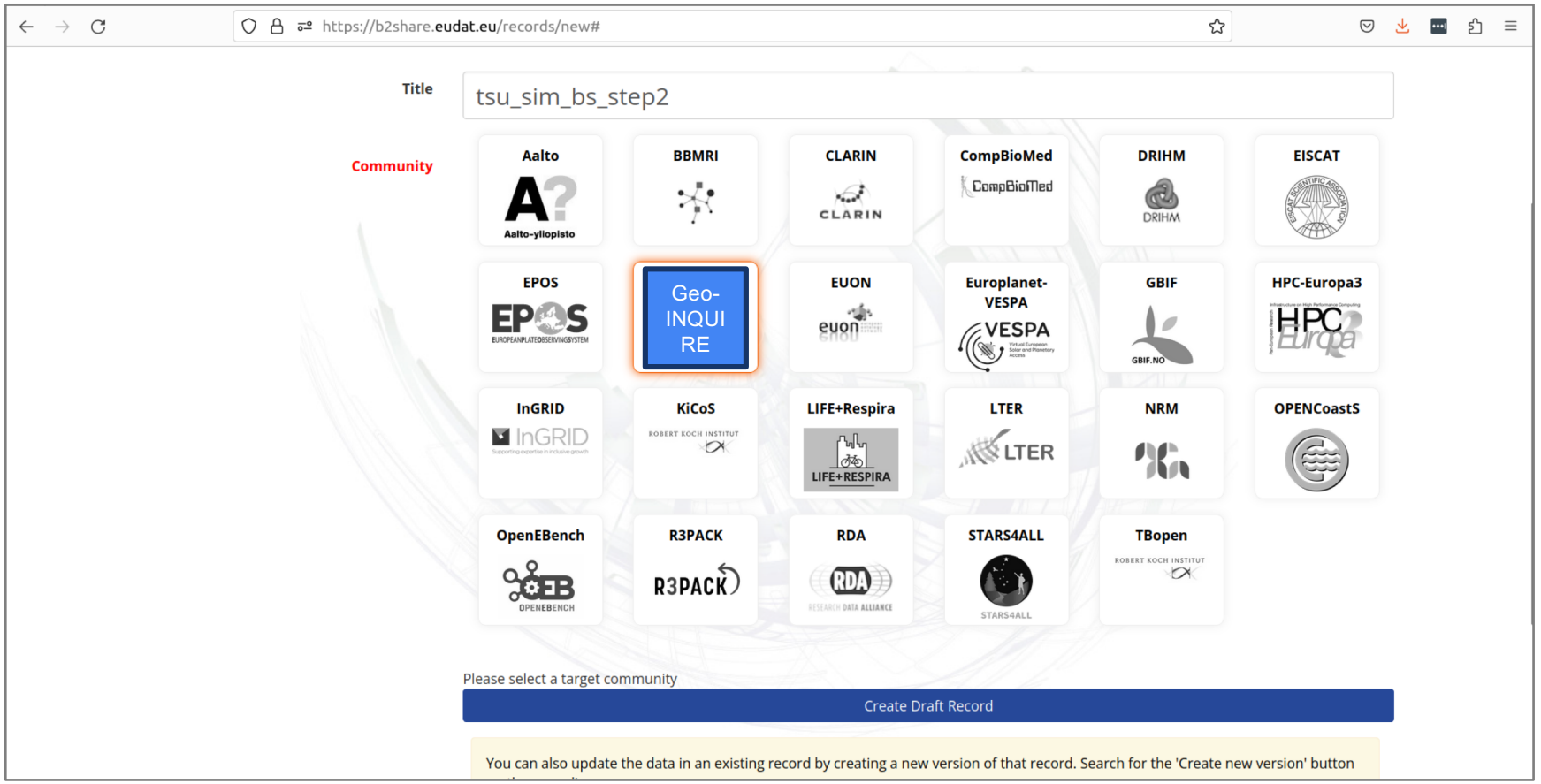
Geo-Inquire community created in B2SHARE



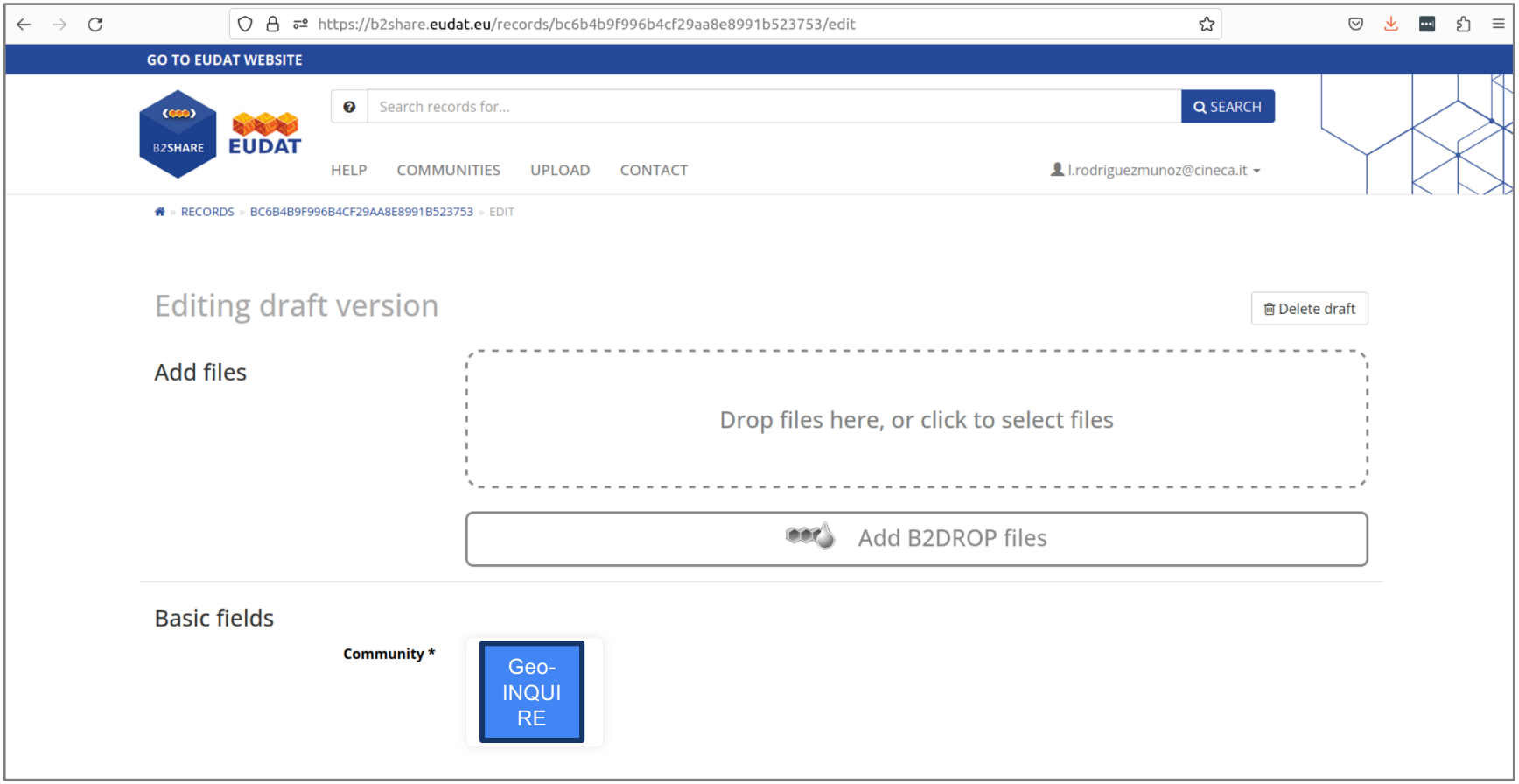
B2SHARE demo: Communities



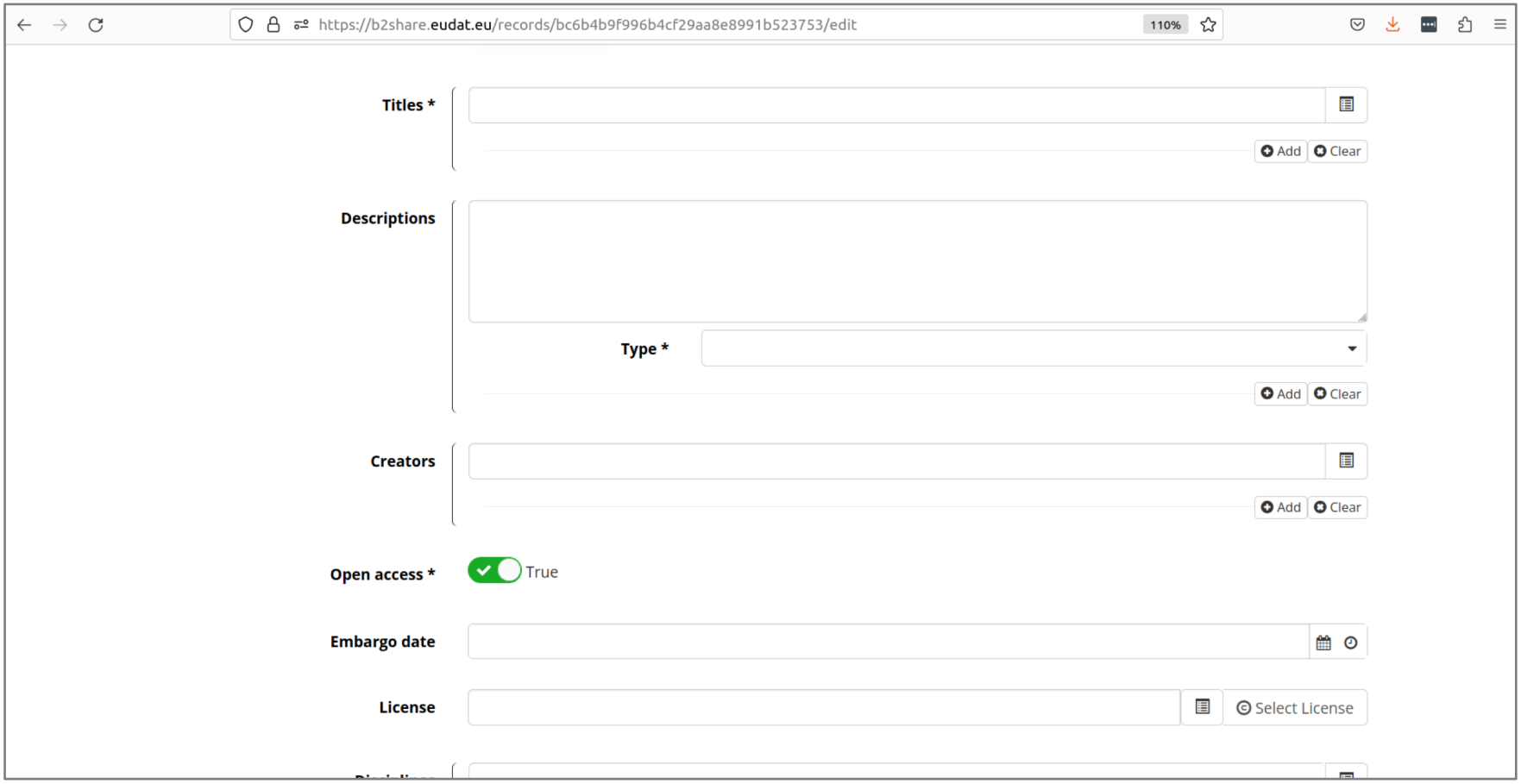
B2SHARE demo: Upload dataset



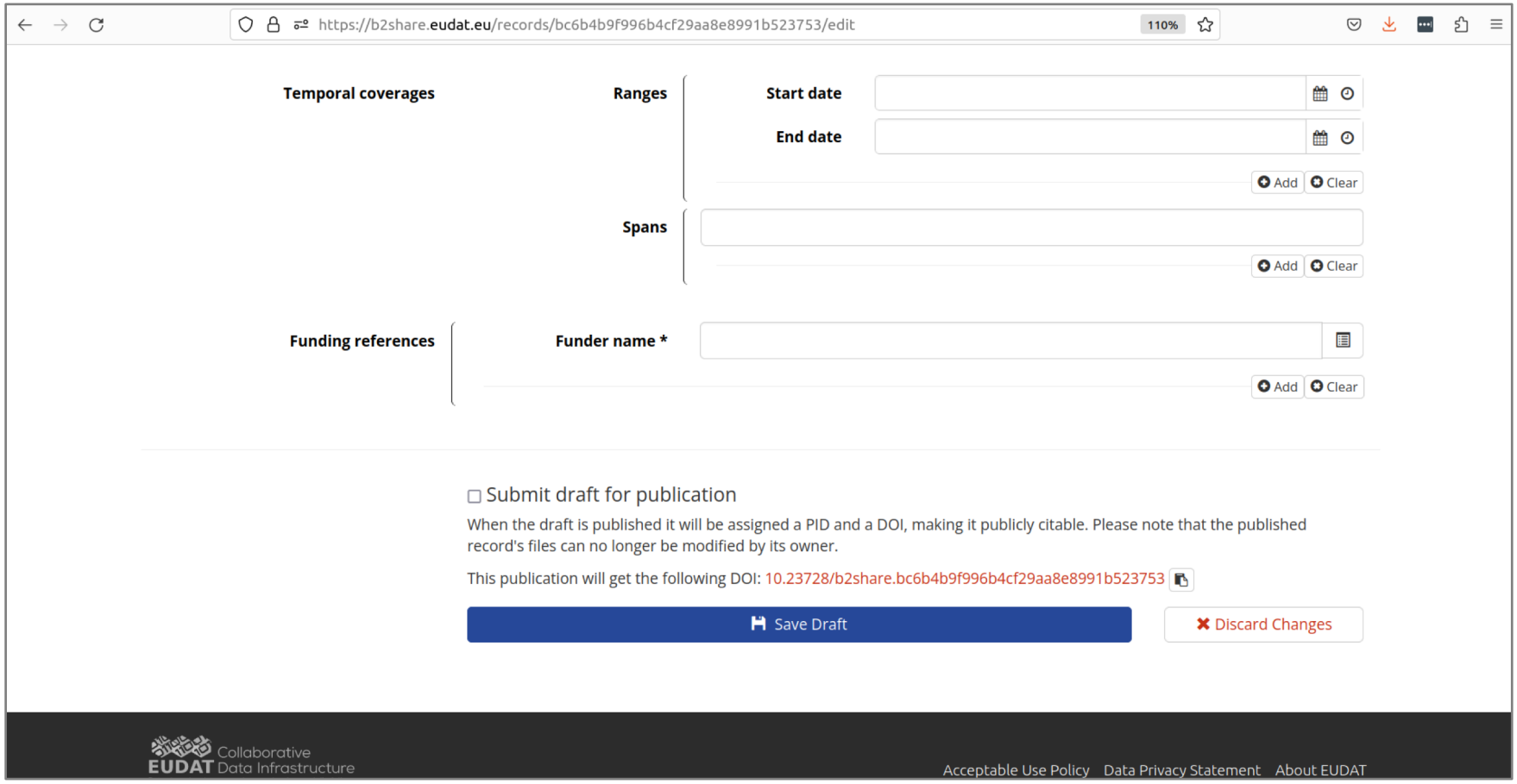
B2SHARE demo: Load files



B2SHARE demo: Metadata (general + community)



B2SHARE demo: Save draft or publish directly



B2SHARE | EUDAT Extended Metadata Schema

(https://schema.eudat.eu/eudatcore_metadataelements/)

Metadata elements:

- Community (O)
- Title (M)
- Description (R)
- Keywords (R)
- Identifier (M)
- RelatedIdentifier (O)
- Creator (R)
- Publisher (M)
- Contributor (O)
- Instrument (O)
- PublicationYear (M)
- Language (R)
- Contact (O)
- Rights (R)
- ResourceType (O)
- Format (O)
- Size (O)
- Version (O)
- FundingReference (O)
- Discipline (O)
- Spatial Coverage (O)
- Temporal Coverage (O)

The Extended MD schema can be further customised adding elements community specific

Next Steps

Simulation Data are:

- BIG: in Geo-Inquire dataset size of the order of 10-30 TB
- HPC proximity important, not easy to move the data
- Easy sharing of data with the HPC-CLOUD-IAC
- In Cineca we are providing tools for visualisation, Interactive Computing, and more
- Extraction of data from single datasets and files

SDL to become the archive for the data assets
in the geoscience community
also supporting the Digital Twins

Next Steps

At CINECA we are assessing the possibility of **developing a Data Lake solution based on:**

Object-storage and cloud-native technologies:

- High availability and fault tolerance.
- Scalable.
- Updating/maintenance is easier.

- It can potentially be integrated with S3 compatible storage systems in other computing centers or research institutions.

- Early stage of design.

Thank you!

Geo-INQUIRE is a joint effort of 51 institutions

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Dataset example

- Tsunami simulations from INGV: Experiment_Samos.
- 40000 scenarios (simulation runs).
- There's a folder for each scenario.
- Input is grouped in a folder.
- Subfolders need to be compressed.
- JSON metadata (EUDAT Core Schema).
- User needs to download sim_setup and any single simulation to be able to reproduce it.

```
Experiment_Samos
├── BS_scenario00001
│   ├── out_ts.nc
│   ├── out_ts_ptf.nc
│   └── parfile.txt
├── BS_scenario00002
│   ├── out_ts.nc
│   ├── out_ts_ptf.nc
│   └── parfile.txt
├── BS_scenario00003
│   ├── out_ts.nc
│   ├── out_ts_ptf.nc
│   └── parfile.txt
├── BS_scenario00004
│   ├── out_ts.nc
│   ├── out_ts_ptf.nc
│   └── parfile.txt
├── BS_scenario00005
│   ├── out_ts.nc
│   ├── out_ts_ptf.nc
│   └── parfile.txt
└── sim_setup
    ├── Step1_scenario_list_BS.txt
    ├── Step2_extract_ts.py
    ├── Step2_local_domain_2020_1030_samos.grd
    ├──Step2_local_domain_2020_1030_samos_POIs_deth.dat
    └── Step2_ts.dat
```