swissuniversities

National policy and support actions for research data skills: Impact & Experiences

University use cases & experiences on developing RDM & FAIR data skills

Dr. Aude Bax de Keating, Open Science Portfolio Manager @ swissuniversities

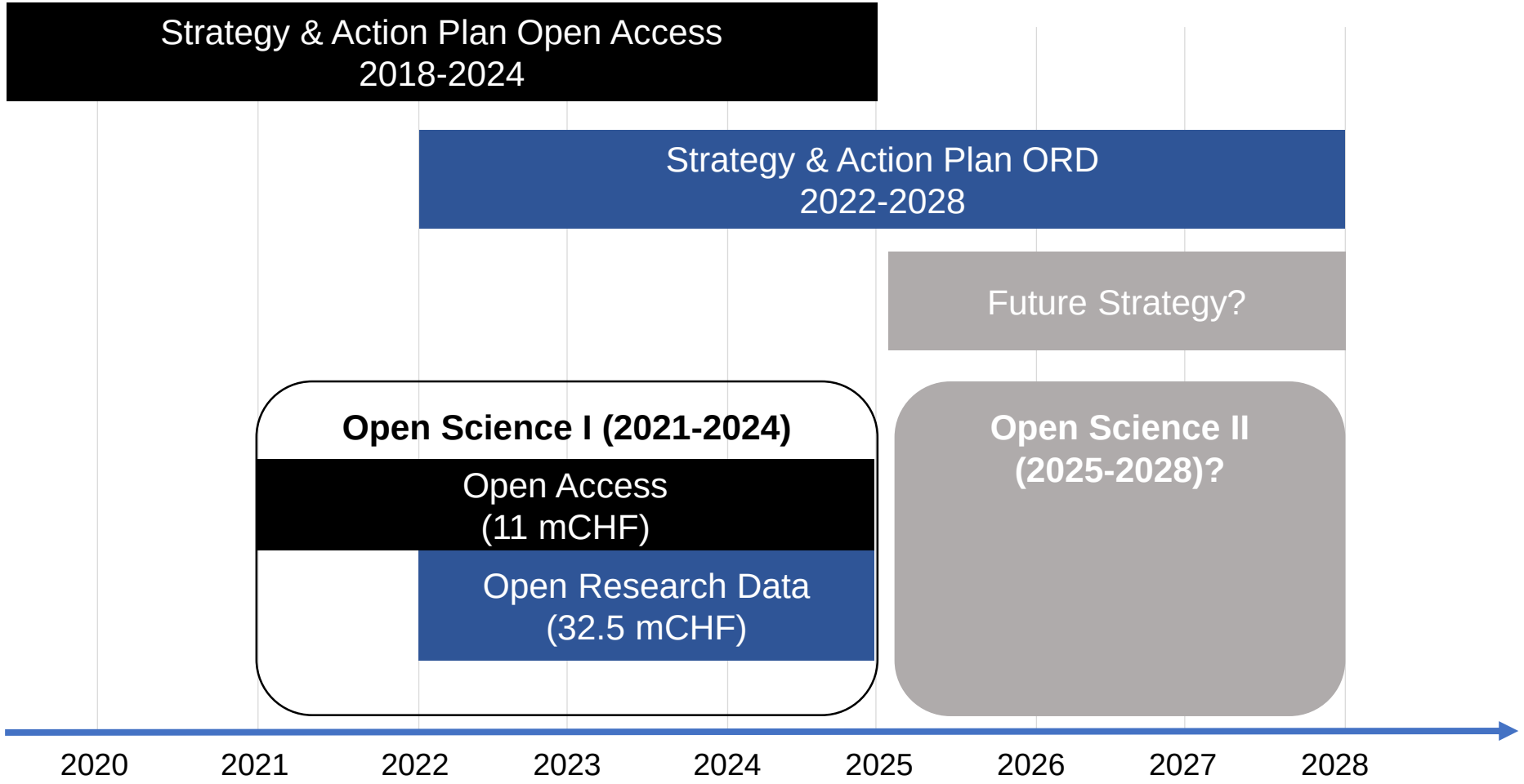
Wednesday April 28, 2021

Online Workshop

RDM & FAIR Data Skills in Switzerland & Beyond

From 3:00 pm to 3:15 pm	
3:00 – 3:02	The Scientific Information & Open Science Programs @ swissuniversities, Dr. Aude Bax de Keating
3:02 – 3:06	Tools & Services for FAIR RDM at ETH Zurich, Dr. Henry Lütcke
3:06 – 3:10	DLCM & OLOS, UNIGE, Dr. Pierre-Yves Burgi
3:10 – 3:15	Developing Research Data Skills in Computational Materials Science: AiiDA & Materials Cloud, EPFL Dr. Giovanni Pizzi

The Open Science Programme



Websites: https://www.swissuniversities.ch/en/topics/digitalisation/funded-projects
https://www.swissuniversities.ch/en/topics/digitalisation/open-science

ETH zürich

IT Services

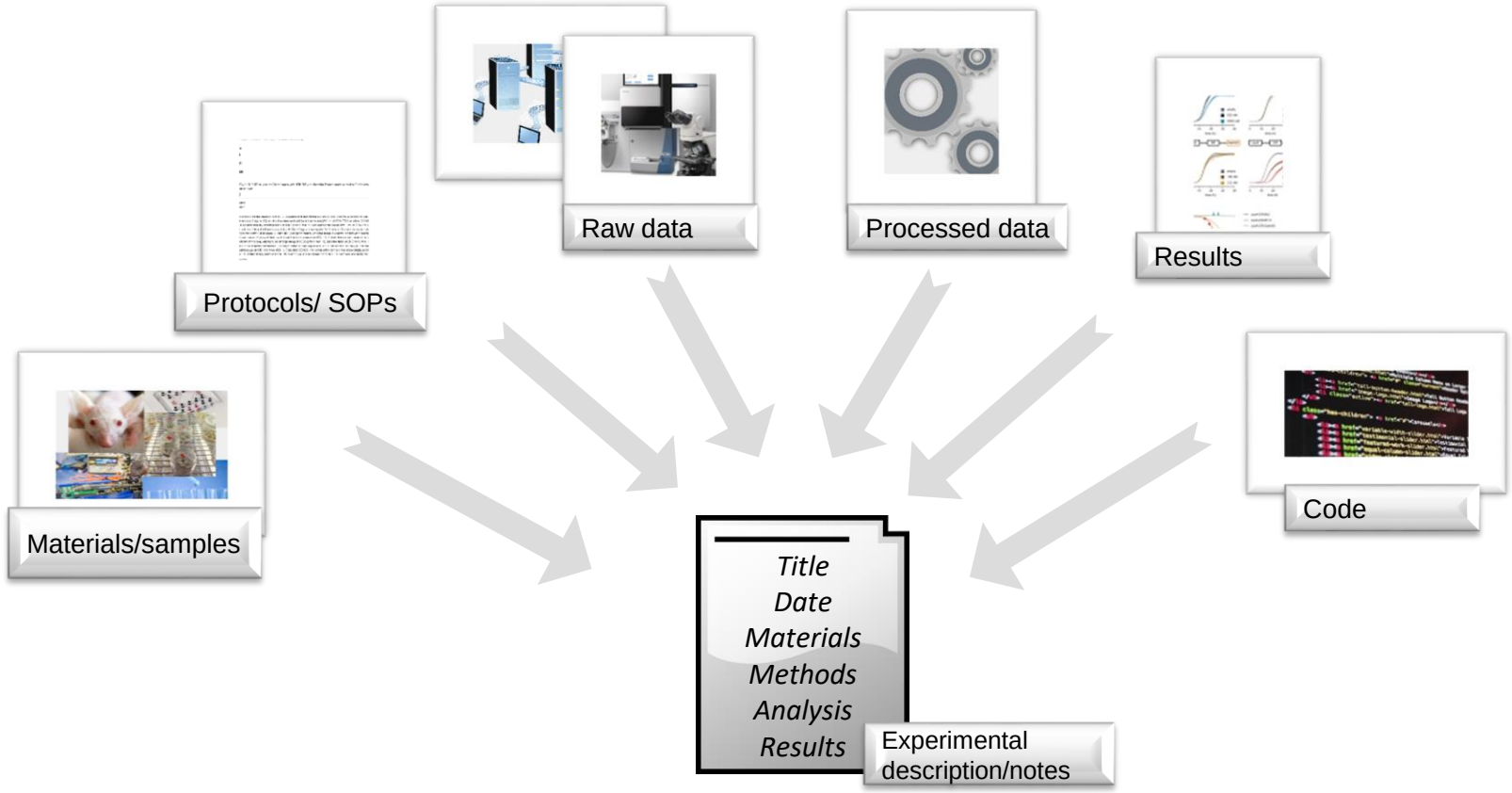
Tools & Services for FAIR RDM at ETH Zurich

28.04.2021

Dr. Henry Lütcke, Scientific Computing Lead
Scientific IT Services, ETH Zurich

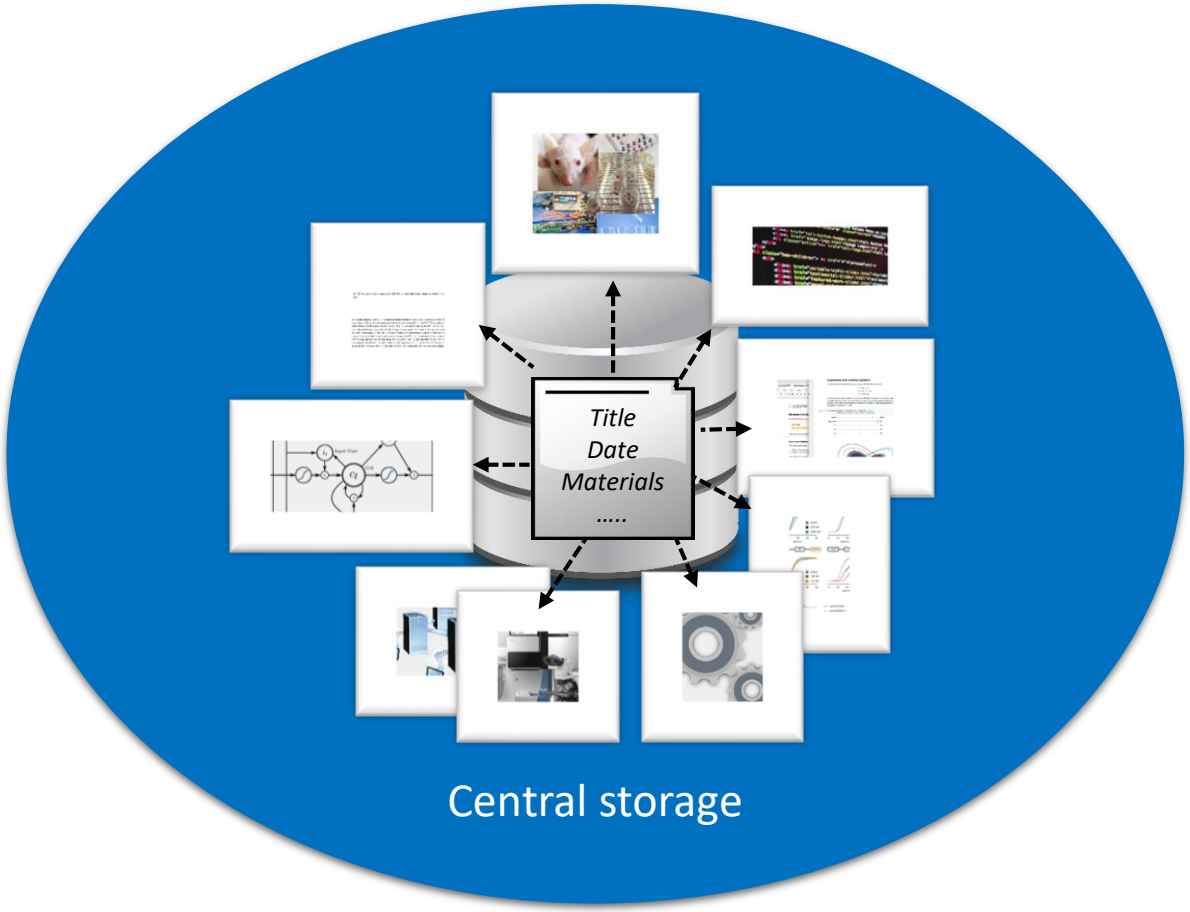
FAIR Data Management

- Funders and journals increasingly demand data publication according to the **FAIR**[1] data principles (**F**indable, **A**ccessible, **I**nteroperable, **R**eusable)
- Making data truly **FAIR involves** tracking and linking **different types of information**



1. **Wilkinson et al.**, *Scientific Data 3, 160018 (2016)*

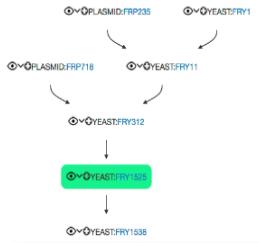
openBIS – Data Management System and Electronic Lab Notebook



openBIS

A combined ELN/LIMS can help make data FAIR

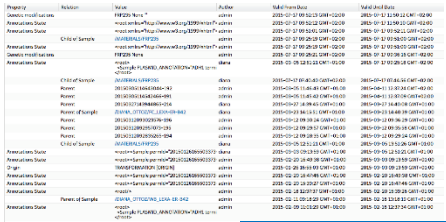
openBIS features



Relationships

Import/Export

User rights management



Audit trail

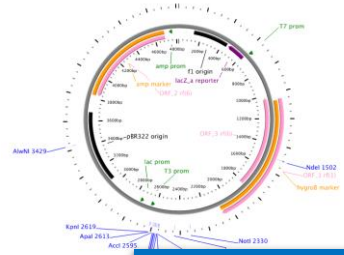
Data immutability

zenodo

ETH zürich
Research Collection

Data Repository Integration

BLAST search



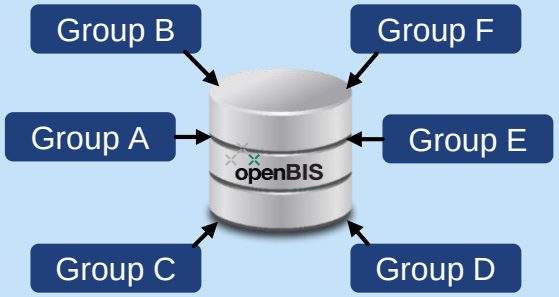
Plasmid maps

https://openbis.ch

RDM Services based on openBIS

- openBIS **source code is freely available**: https://sissource.ethz.ch/sispub/openbis
- **Universities and non-profit** research institutes can download **binaries for free**
- ETH SIS offers **support services** based on openBIS
- May include **installation, maintenance**, customizations, data modelling or **training & support**

ETH Zürich



- Research Data Nodes
- Research Data Hub
- Training & Consulting

National (CH)

openRDM .swiss

swissuniversities

- Since 2018
- Cloud- or self-hosted
- Training & Support

International

openRDM .eu

EGI

- Since 2021
- Cloud- or self-hosted
- Onboarding & Usage Support

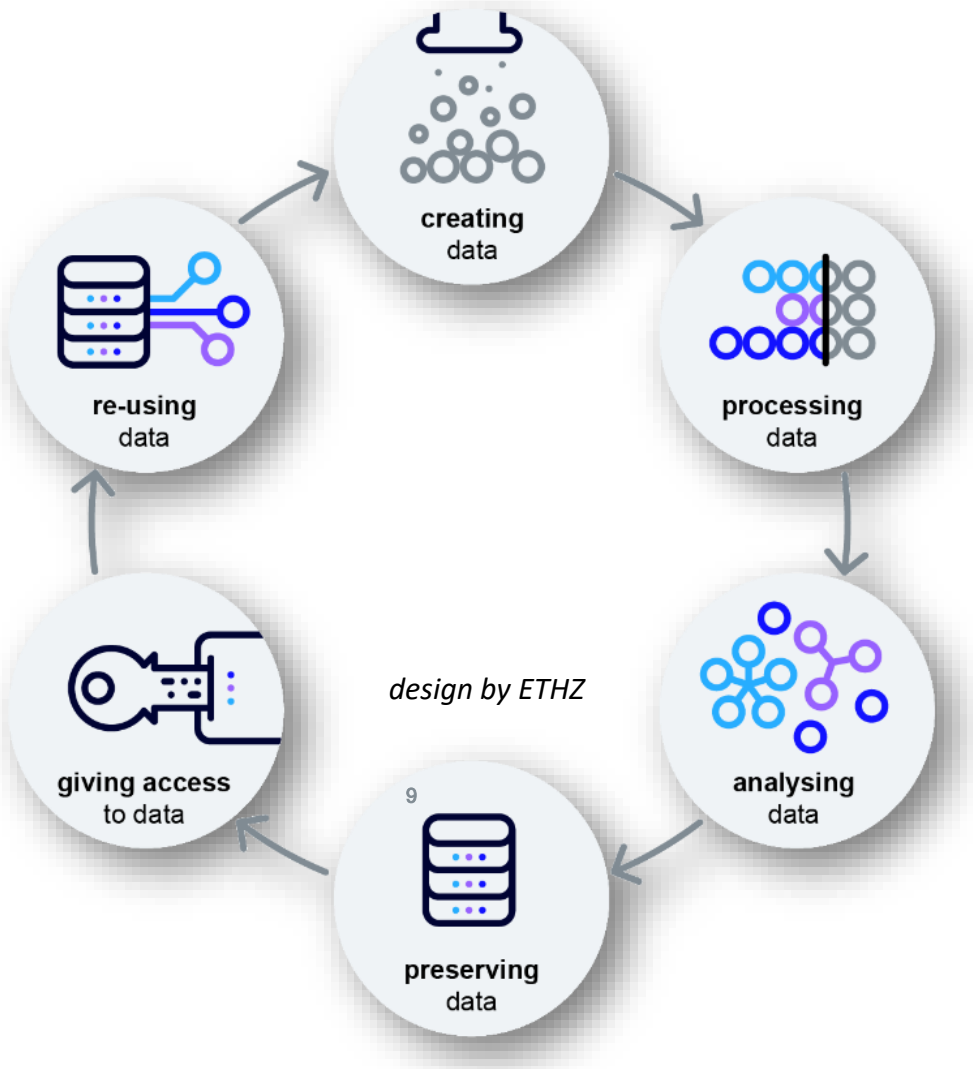
The national DLCM Project 2015-2020

Aug 2015 – Jul 2018: Phase 1
Exploration of the whole life-cycle

Jan 2019 – Dec 2020: Phase 2
From Prototypes to Services

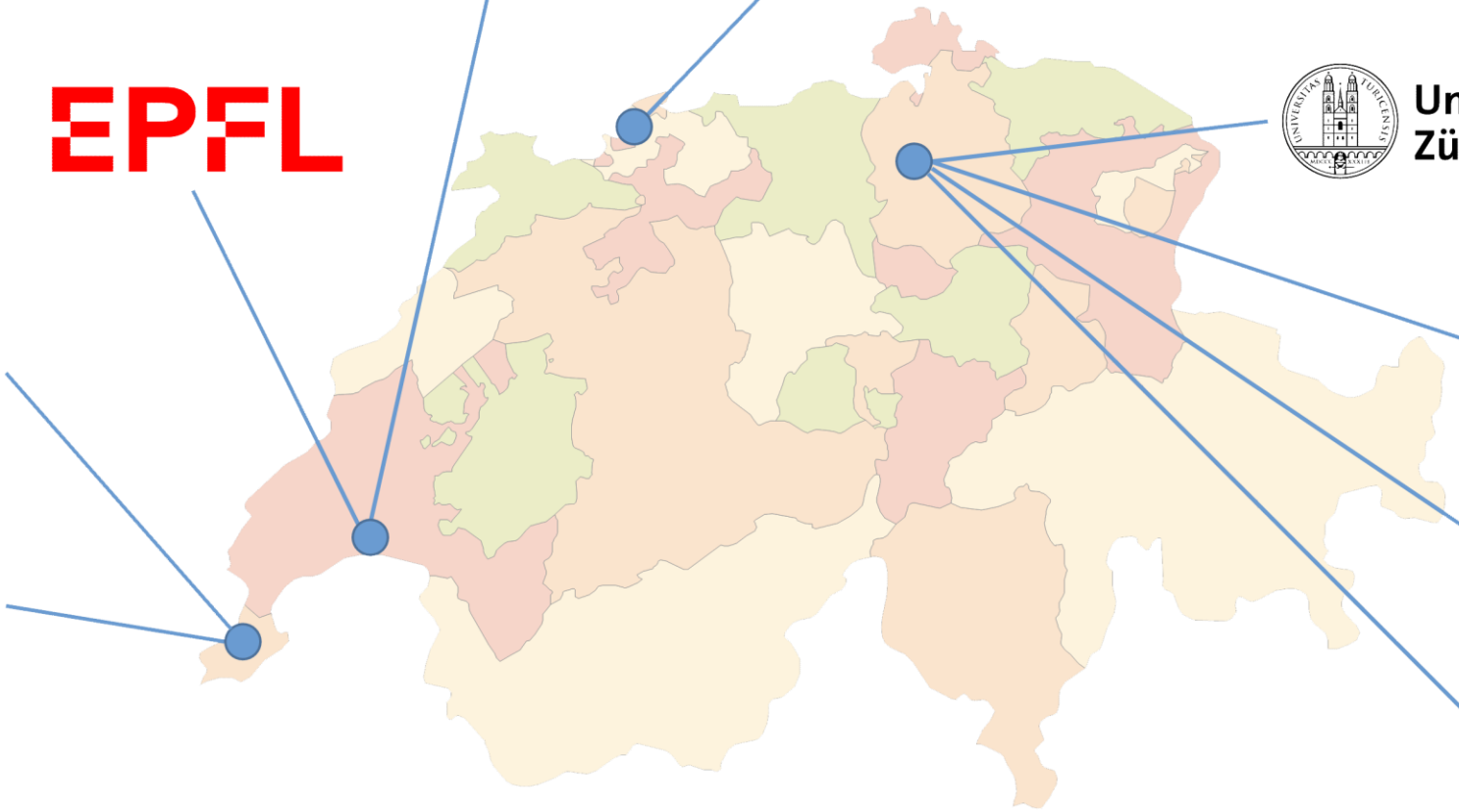
June 2019: YARETA in production
Geneva state's solution

2020: OLOS in production
National solution
2021: OLOS becomes an association



More information at www.dlcm.ch

Partners



UNIL | Université de Lausanne

University of Basel

EPFL

Universität Zürich[UZH]

UNIVERSITÉ DE GENÈVE

ETH zürich

Hes·so
University of Applied Sciences and Arts Western Switzerland

SWITCH

h e g
Haute école de gestion Genève

Zürcher Hochschule für Angewandte Wissenschaften
zh aw

DLCM | Mandated by swissuniversities

OLOS.swiss

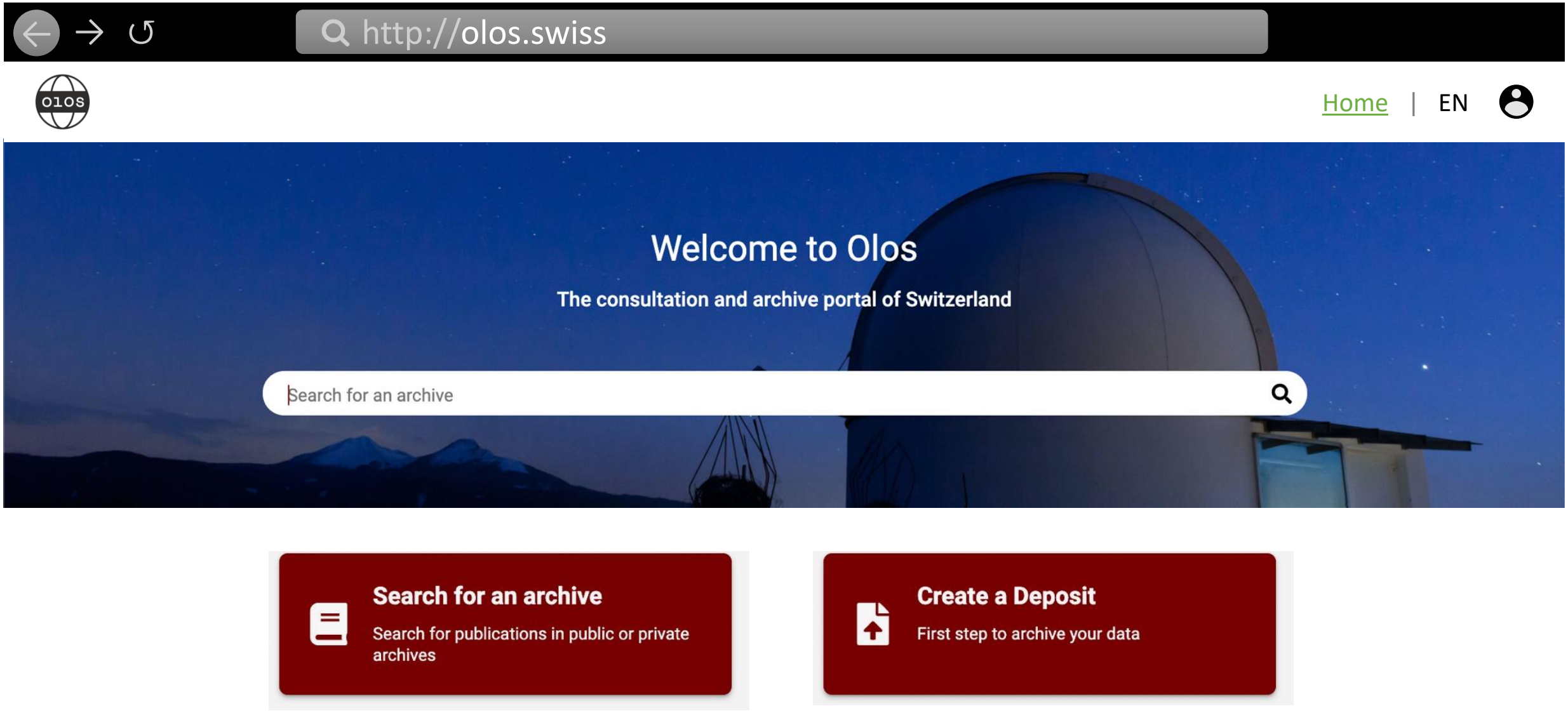
- ✓ Developed as part of the DLCM project
- ✓ Repository for **Swiss researchers**
- ✓ **Swiss-based** servers (original & copy)
- ✓ Compliant with **FAIR principles** & provides a **DOI**
- ✓ **Any format** across all scientific disciplines

Project supported by swissuniversities

&

Non-profit Association

OLOS.swiss


http://olos.swiss
Home | EN
Welcome to Olos
The consultation and archive portal of Switzerland
Search for an archive
Search for an archive
Search for publications in public or private archives
Create a Deposit
First step to archive your data

OLOS.swiss

EASY AND USEFUL FEATURES

- ✓ Control access to your data
- ✓ Define your data retention period, licenses, etc.
- ✓ Choose your workflow, with or without validation
- ✓ Keep your folder structure

COMPLIANT WITH POLICIES

- ✓ Complies with Swiss law
- ✓ Follows FAIR principles
- ✓ Assigns a persistent identifier (DOI)
- ✓ Eligible for funding from the SNSF for data upload
- ✓ Complies with 12 open and international standards, protocols, and registries

SUITABLE TO YOUR NEEDS

- ✓ Try it yourself!
- ✓ Consulting & Training: Receive customized assistance for large datasets, etc.
- ✓ Customize the metadata schema to your field
- ✓ Integrate OLOS to your research environment

Consulting & Training Activities

Annual program for training session in collaboration with DevPro HESSSO

DMP coaching

Tools, guides, practical sources, documents customized tools

On demand trainings in different discipline

RDM Mooc & on demand e-learning session

RDM Certification

Available by the end of 2021 !

olos.swiss

QUESTIONS?

DLCM 2.0 | Mandated by swissuniversities

Website https://www.dlcm.ch/olos

Contact us > olos.swiss/contact

Integrate with your lab equipment

- DLCM integration guide > https://sandbox.dlcm.ch/administration/docs/DLCM-IntegrationGuide.html

Sign up for our newsletter > olos.swiss/newsletter/register

UNI FR UNIVERSITÉ DE FRIBOURG UNIVERSITÄT FREIBURG

heg Haute école de gestion Genève

Hes·so Haute Ecole Spécialisée de Suisse occidentale

UNIVERSITÉ DE GENÈVE

Developing Research Data Skills in Computational Materials Science: AiiDA and Materials Cloud

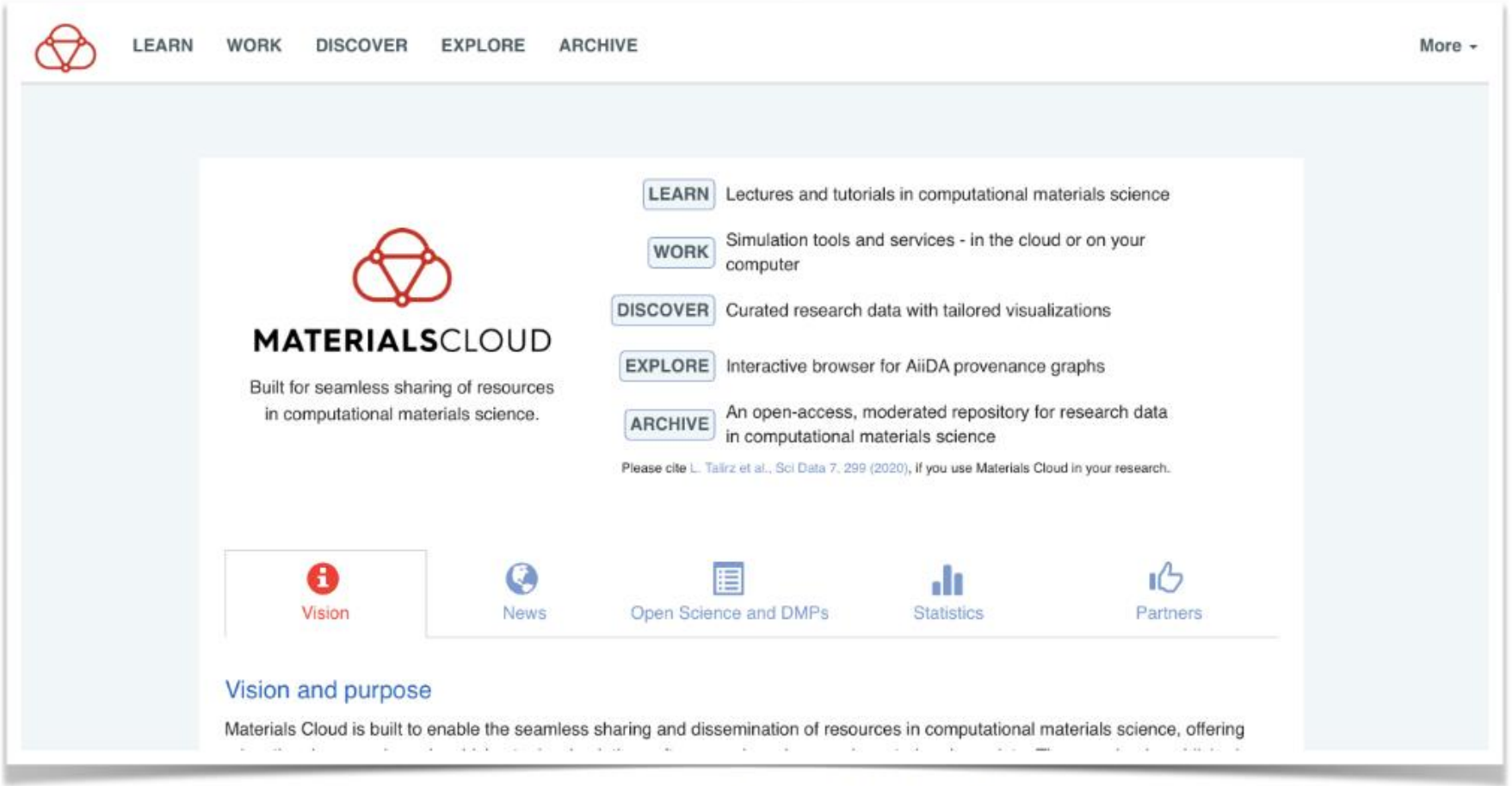
Giovanni Pizzi

Theory and Simulation of Materials (THEOS)
National Centre for Computational Design and Discovery of Novel Materials (MARVEL)

EPFL, Switzerland

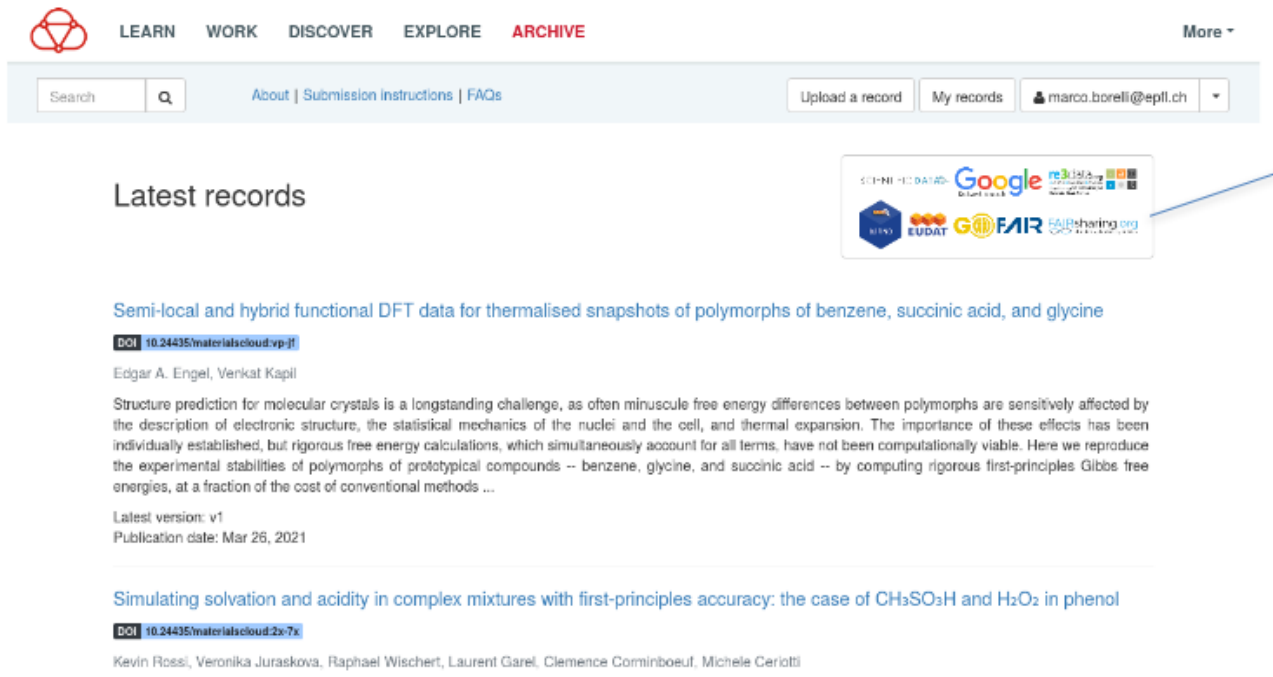
www.materialscloud.org

- A portal for research data dissemination and cloud simulations



L. Talirz et al., Sci Data 7, 299 (2020)

Materials Cloud Archive: a repository for data sharing



Indexed by Google Dataset Search and by EUDAT/EOSC's B2FIND

Registered on FAIRsharing.org and re3data.org

- Releases DOIs for data associated to papers, open to the world
- Based on CERN's Invenio v3

Recommended by Nature's journal "Scientific Data"

SCIENTIFIC DATA

https://www.nature.com/sdata/policies/repositories#materials

New! Recommended by the new "Open Research Europe" journal

European Commission

Research and Innovation

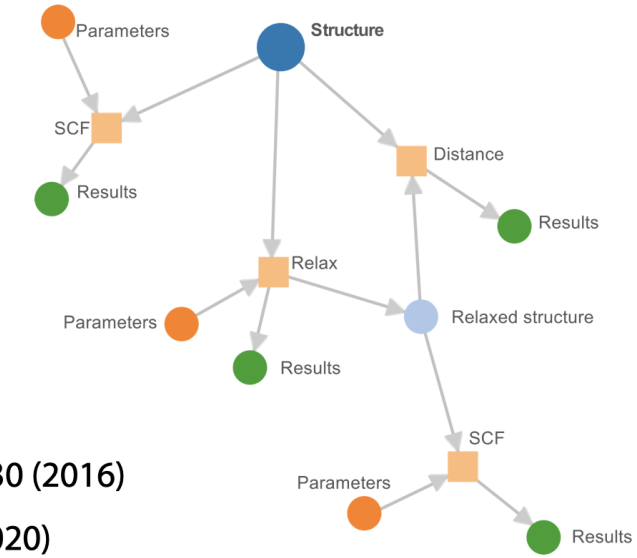
Open Research Europe

https://open-research-europe.ec.europa.eu/for-authors/data-guidelines

Providing tools for reproducible research

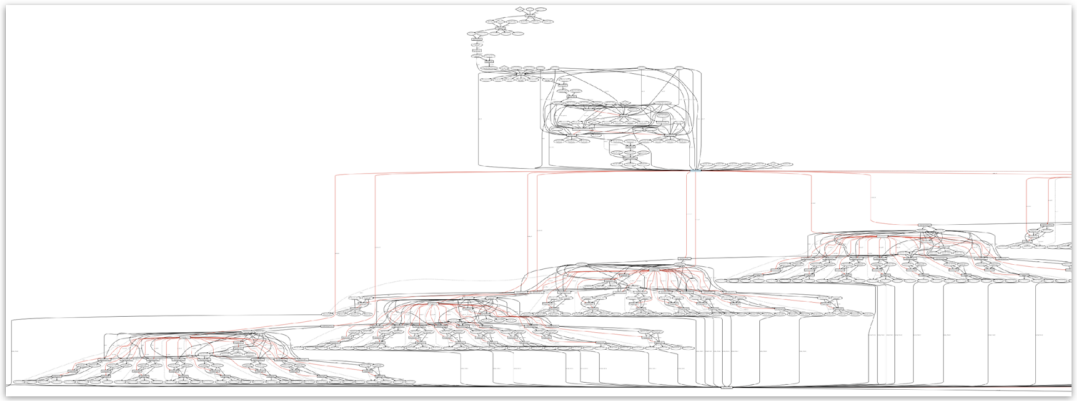
AiiDA

http://www.aiida.net



G. Pizzi et al., Comp. Mat. Sci. 111, 218-230 (2016)

S.P. Huber et al., Scientific Data 7, 300 (2020)



Molecular dynamics study of lithium in a solid electrolyte

- Computational science infrastructure to automate high-throughput simulations, locally and on HPC resources
- Track automatically **provenance graphs**: full reproducibility
- Plugin interface
- Facilitate managing simulations with appropriate data management
- Work in progress to integrate with openBIS for experiments

AiiDA PLUGIN REGISTRY

Registered plugin packages: 58

Calculations	98 plugins in 39 packages
Parsers	84 plugins in 40 packages
Data	79 plugins in 24 packages
Workflows	95 plugins in 27 packages
Console scripts	19 plugins in 14 packages
Other	95 plugins in 26 packages

Interoperability, Standards, APIs: OPTIMADE

OPTIMADE
Open Databases Integration for Materials Design

http://www.optimade.org

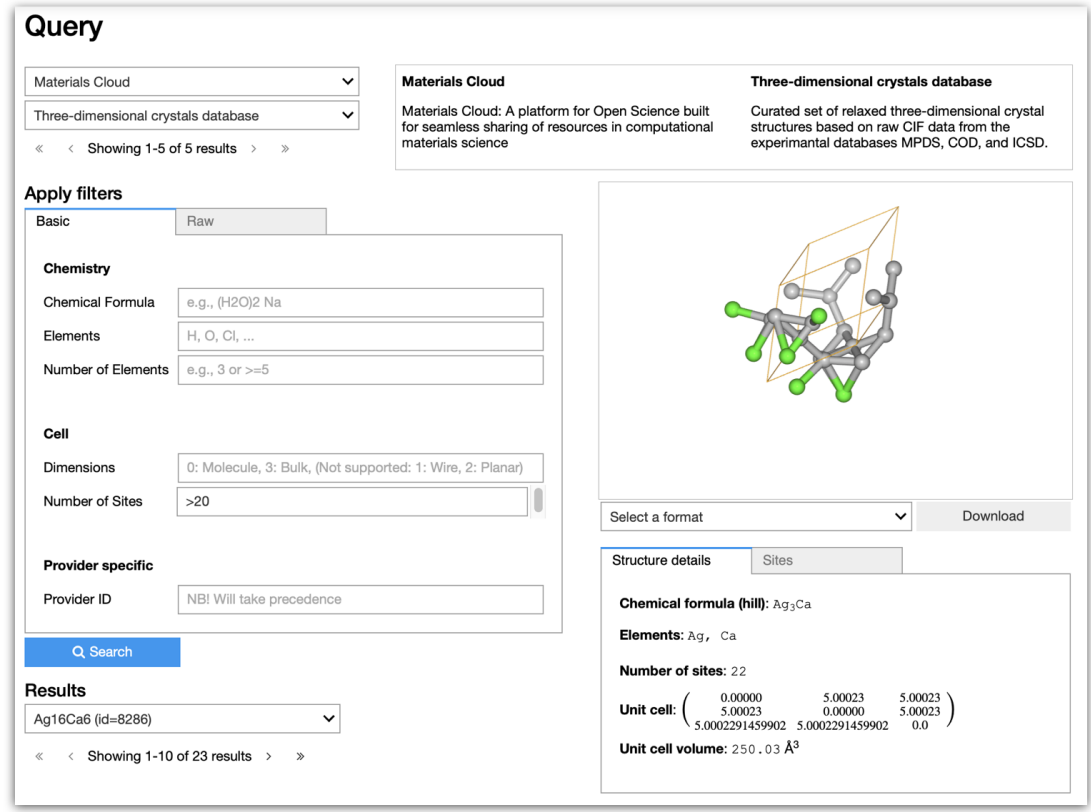
C. W. Andersen et al., arXiv:2103.02068 (2021)

Standard REST API to search for crystal structures in 10+ different databases

Provider: Materials Cloud data available via OPTIMADE

Client: client available on Materials Cloud: get data from any compliant server

Client connected with cloud simulations: quickly launch a calculation from a structure

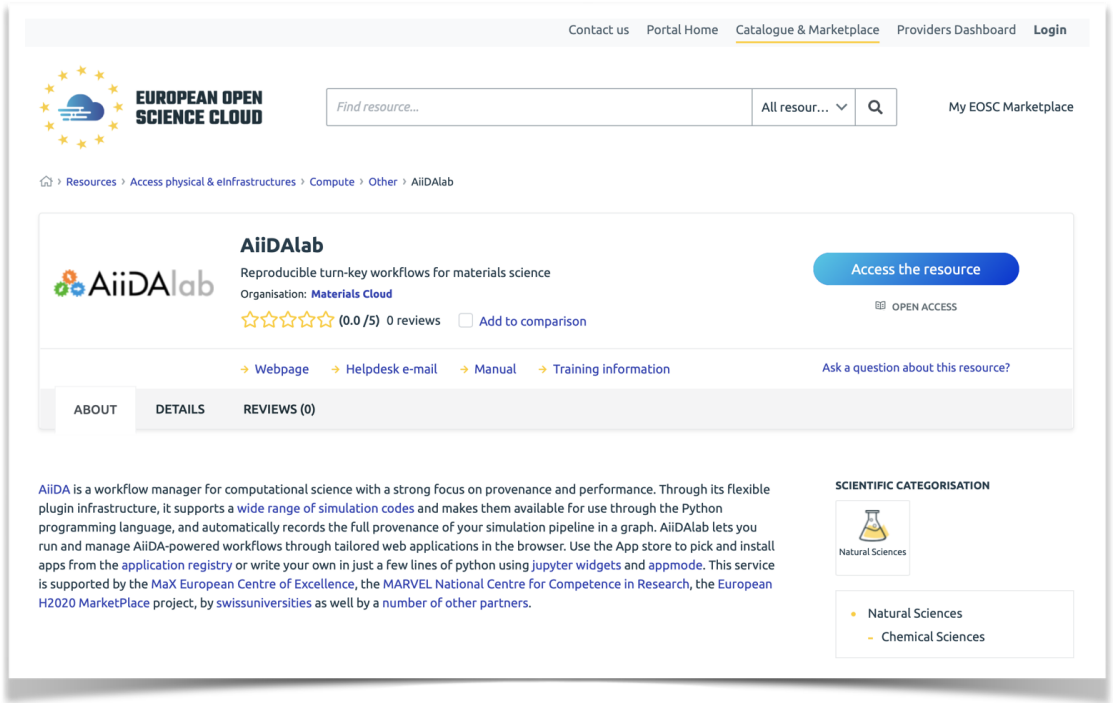


https://www.materialscloud.org/optimadeclient

Availability on the EOSC Marketplace

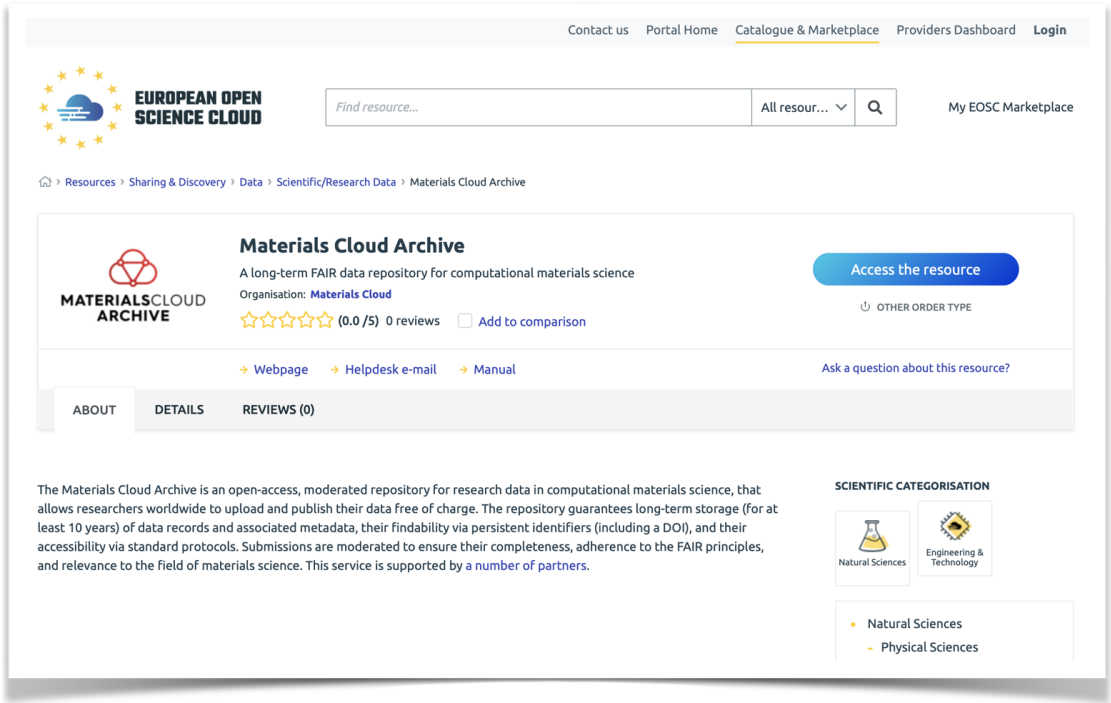
Two of the services we provide are available on the EOSC Marketplace to all researchers

Cloud simulations



https://marketplace.eosc-portal.eu/services/aiida-lab

Repository and long-term storage



https://marketplace.eosc-portal.eu/services/materials-cloud-archive

Simplifying researchers's life: Data Management Plan templates

Data Management Plan

In order to support researchers using the Materials Cloud to prepare grant applications or to comply with agencies' requirements, we provide here below templates for data management plans (DMPs) that use the Materials Cloud.

Dissemination can be as simple as depositing data freely (and in any format) on the Archive, or, if using AiiDA, disseminating entire workflows, raw and curated data in the Explore or Discover sections. AiiDA plugins and workflows can also be distributed trrough the AiiDA plugin repository, while simulation services can be exposed through AiiDAlab, either in a virtual machine environment (the Quantum Mobile) or on the cloud (e.g. on the European Open Science Cloud).

Feel free to contact us with any questions regarding the use of the Materials Cloud Archive as part of your data management plan.

Funding Body	DMP template (using AiiDA)	DMP template (no AiiDA)
SNF	.docx .odt .pdf	.docx .odt .pdf
H2020	.docx .odt .pdf	.docx .odt .pdf

Please also note the resources provided by EPFL, including extensive DMP templates for many different project types (SNSF, ERC, H2020, ...).

Materials Cloud fulfils the requirements for data repositories

The Materials Cloud Archive fulfils the SNF requirements for data repositories.

- **Non-commercial:** Yes, all backing institutions are non-profit
- **Usage of globally unique and persistent identifiers:** Yes, uses DOI as permanent identifier system

H2020 DMP Template

This is a data management plan (DMP) template for a H2020 project in computational materials science using the Materials Cloud Archive as a data repository and AiiDA to collect the full provenance of the calculations performed.
If you have any feedback or questions feel free to contact us at info@materialscloud.org.

Further H2020 guidelines on DMPs can be found here.

Please adapt the template to your project!

1. Data Summary

- What is the purpose of the data collection/generation and its relation to the objectives of the project?
- What types and formats of data will the project generate/collect?
- Will you re-use any existing data and how?
- What is the origin of the data?
- What is the expected size of the data?
- To whom might it be useful ('data utility')?

The *ab initio* calculations performed in this project are expected to generate large volumes of data, most of it is in the form of intermediate binary files, which can be straightforwardly regenerated from the original inputs.

In this project, calculations will be performed through the *Automated Interactive Infrastructure and Database for Computational Science* (AiiDA), a python framework for high throughput calculations and provenance tracking (www.aiida.net). AiiDA automatically stores all information required to reproduce the result of each calculation. On the output side, AiiDA is designed to strike a balance between the cost of storage and the cost of recomputing a piece of data. For example, by default, total energies, electronic band structures and log files are stored, while Kohn-Sham wave functions and charge densities are not.

Before submitting a calculation through AiiDA, all inputs (+ metadata, see 2.1) are automatically stored in a local database. AiiDA then transmits the necessary information to the target computer, which can be a remote supercomputer, a local cluster or the workstation of the researcher. AiiDA adds the calculation to the computer's job queue, monitors the status, and retrieves the results once the calculation is finished.

In this model, all data is generated on the target computer, while only the data intended for preservation is transferred back to the workstation of the researcher.

https://www.materialscloud.org/dmp

Training events (tutorials, workshops)

https://www.aiida.net/events/

Events

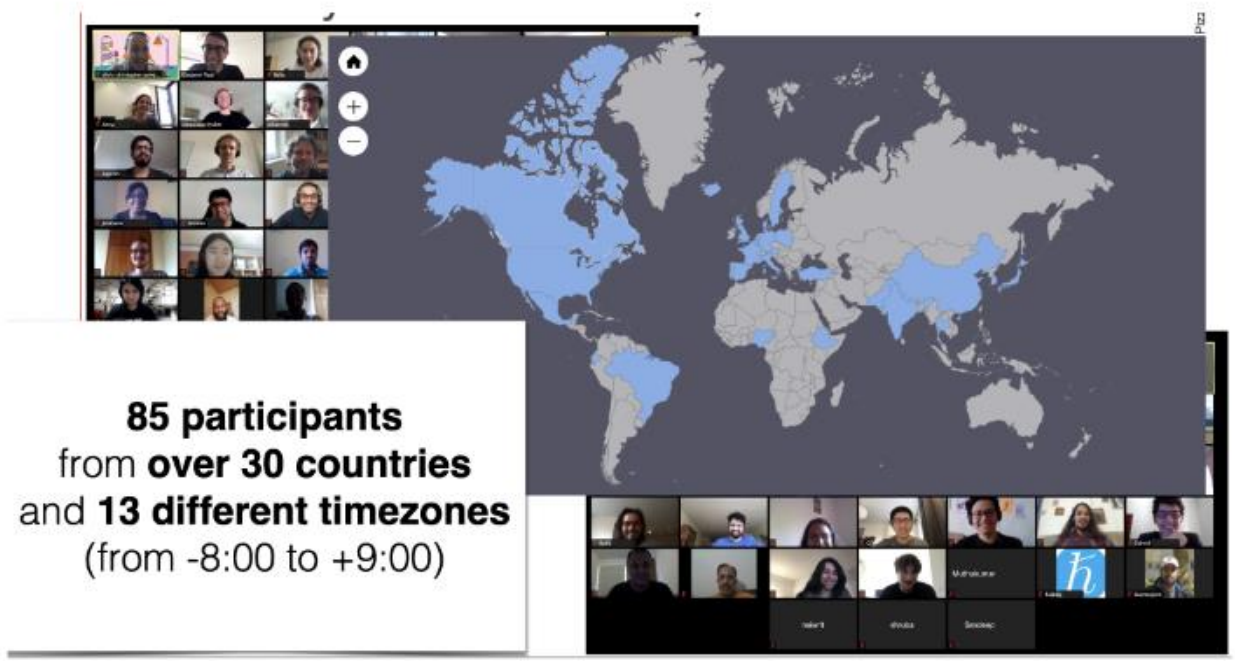
Upcoming events

- **(Tentative) [Week of July 6th, 2021]** Online AiiDA tutorial for all timezones

Past events

- **[10 Feb 2021]** AiiDA tutorial at the Federal University of ABC, São Paulo – Brazil, with ~20 participants.
- **[2 Dec 2020]** AiiDA tutorial at the BIG-MAP workshop with ~80 participants (event site)
- **[10 July 2020 – 4 pm CT]** Materials Science Q&A @ SciPy 2020 (event site)
- **[9 July 2020 – 5 pm CT]** AiiDA talk @ SciPy 2020 (event site)
- **[7-10 July 2020]** AiiDA virtual tutorial week, sponsored by MARVEL, MaX, CECAM, swissuniversities and MarketPlace. Introductory presentations and hands-on workshops for ~80 participants (event site, tutorial material, report)
- **[Oxford (UK) 25-27 March 2020]** Introduction to AiiDA, aiida-wannier90 plugin, and the workflows to compute automatically Wannier functions within the School "Wannier90 v3.0: new features and applications" with ~40 participants (event site) (slides, material and video recordings)
- **[CINECA Bologna (IT) 17-21 February 2020]** Hackathon on plugin and workflow development for AiiDA with ~25 participants (event site)
- **[ISSP University of Tokyo (JP) 19-20 December 2019]** AiiDA tutorial (tutorial site)
- **[Fiesch (CH) 9-13 December 2019]** Fourth annual AiiDA coding week with ~15 participants (event site)
- **[IIT Mandi (IN) 9-11 October 2019]** Writing reproducible workflows for computational materials science using AiiDA (tutorial site)
- **[SINTEF Oslo (NO) 23-27 September 2019]** VASP & AiiDA workshop (tutorial site)
- **[Ljubljana, 16-20 September 2019]** AiiDA tutorial within the summer school on *Advanced Materials and Molecular Modelling with Quantum ESPRESSO (QE-2019)*.
- **[Xiamen University (CN) 6 September 2019]** Introduction to AiiDA 1.0 (as part of a workshop on computational chemistry and machine learning)
- **[EPF Lausanne (CH) 21-24 May 2019]** Writing reproducible workflows for computational materials science, using AiiDA 1.0 (with >50 participants)
- **[EPF Lausanne (CH) 25-29 Mar 2019]** AiiDA plugins migration workshop, to support

- Training on tools to facilitate research data generation
- Specific sessions on research data management
- Inclusive, duplicated to cover all timezones



85 participants
from **over 30 countries**
and **13 different timezones**
(from -8:00 to +9:00)

Results from July 2020 virtual tutorial