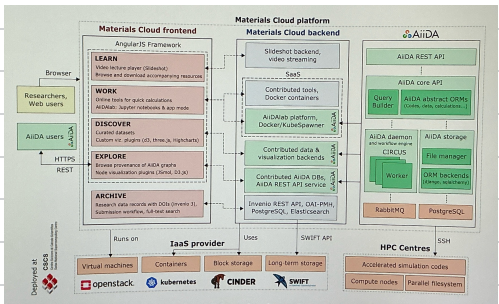


Materials Cloud, a platform for open computational science

- FAIR: findable, accessible, interoperable, reusable
- open science platforms aim to replicate the publicity of platforms that share source code (i.e. github, bitbucket, gitlab)
 1. support + adopt open-source simulation codes/analytic tools;
 2. provide open-souce framework for defining/managing comp. workflows;
 3. offer turnkey solutions from open-source workflows and curated open datasets;
 4. enable FAIR sharing of data and workflows
- Material cloud: learn, work, discover, explore, archive

Section	Content	Target audience	Objective	Access	Submission
LEARN	Video lectures and tutorials	Students and experts in computational materials science	Dissemination of educational and research content	Open, no registration	Partners; other submissions considered
WORK	Online simulations tools and services; redeployable locally	Researchers in computational materials science	Dissemination of open simulation services and tools	Open, with registration for AiiDALab	Partners; other submissions considered
DISCOVER	Curated datasets of calculated materials properties	Researchers in materials science	Dissemination of calculated materials properties	Open, no registration	Partners; other submissions considered
EXPLORE	AiiDA databases and their graphs	Researchers in computational materials science; data scientists	Exploration and query of the raw data and provenance of AiiDA workflows	Open, no registration	Open, with registration
ARCHIVE	Computational data in any format; experimental data linked to computational data	Researchers in materials science; data scientists	FAIR research data dissemination and storage	Open, no registration	Open, with registration

- large focus on reproducibility
- AiiDA: automated workflows for computational science
- Jupyter notebooks contain instructions for AiiDA workflow manager —> interactive web apps.
- Data preservation highlighted for Materials Cloud, even after the research funding is depleted
- Modular architecture



This paper discusses the platform Materials Cloud and its role as an “open-science” platform. It aims to follow the FAIR method of computational science as well as prolonging data longevity. The platform acts in a way which is similar to GitHub in which it is a centralized system for data storage whilst easily accessible to the public.