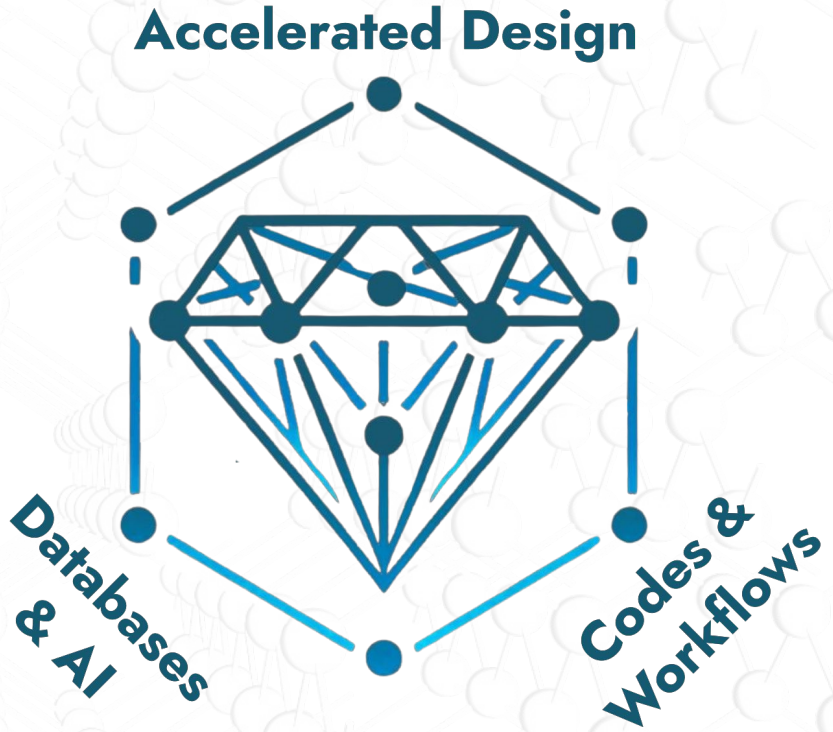
DIAMOND

Codes and Workflows



DIAMOND : ANR-22-PEXD-0015

Lyon, 14/11/2024

Outline

Diamond-CW Platform

- Presentation and objectives
- Solutions: codes and workflows
- Website DIAMOND + GitLab repository
- Infrastructure of the platform

Highlights

- MOF Learning : workflow use case task 1.4
- LIBELUL : Denoising of RAMAN spectra

Conclusion

Pilotage

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Steering com. D. Rodney (UCBL), A.M. Saitta (SU), T. Deutsch(CEA), P-A. Bouttier (CNRS-UGA)

Recruited Ing. J.P.A. Mendonça (CNRS-UGA), A. Arivazhagan (SU), B. Arrondeau (CNRS-UGA), D. Bissuel (UCBL), J. Daubin (CEA), D. Martin-Calle (UCBL), D. Rolland (CEA)

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MATÉRIAUX ÉMERGENTS

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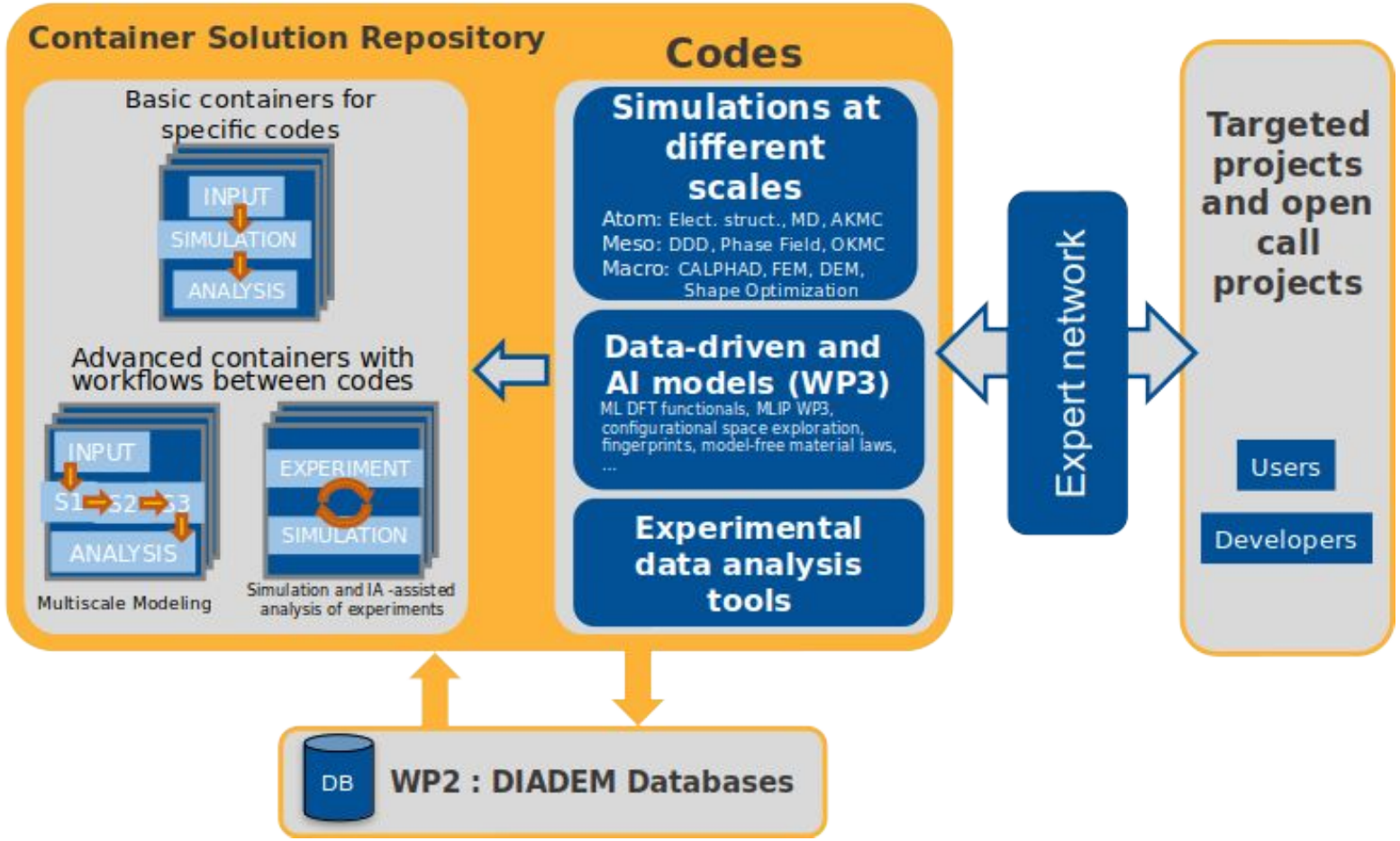
WP1 - General Presentation

- **Containers:** making it easier to install, distribute and use code
- Container **repository**
- **Workflows:** enable code chaining, automation and therefore high throughput, including analysis of experimental data

Meso-center: GRICAD (Grenoble)



Timeline

repo : https://gricad-gitlab.univ-grenoble-alpes.fr/diamond

Empaquetage
comme apt, pip, ...

Guix

Conteneurisation
comme docker, ...

LimeSurvey

Intelligence Artificielle en Sciences des Matériaux

GDR IAMAT

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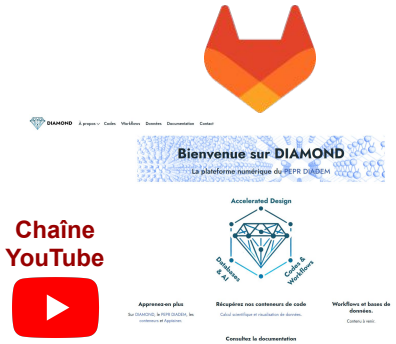
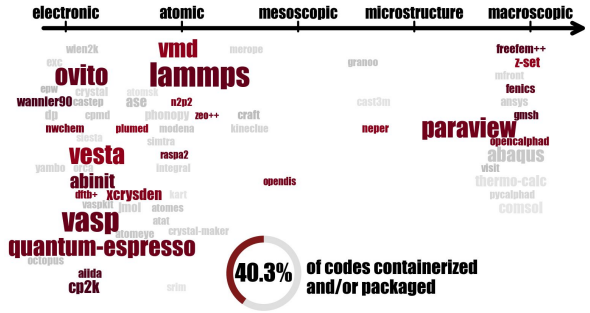
1 AG
DIADÈME

Chaîne YouTube



Site Internet/GitLab



Oct 2023 | Dec 2023 | Feb 2024 | June 2024 | Sept 2024

CMake

python

ASE

MiLaDy

NUMODIS

AiiDA

AMITEX

Lightning-CEGANN

NOM

MOF-LEARNING

iRASPA Molecular Simulations

Zeo++

LIBELUL

DFT-Langevin Dynamics

AiiDA VASP

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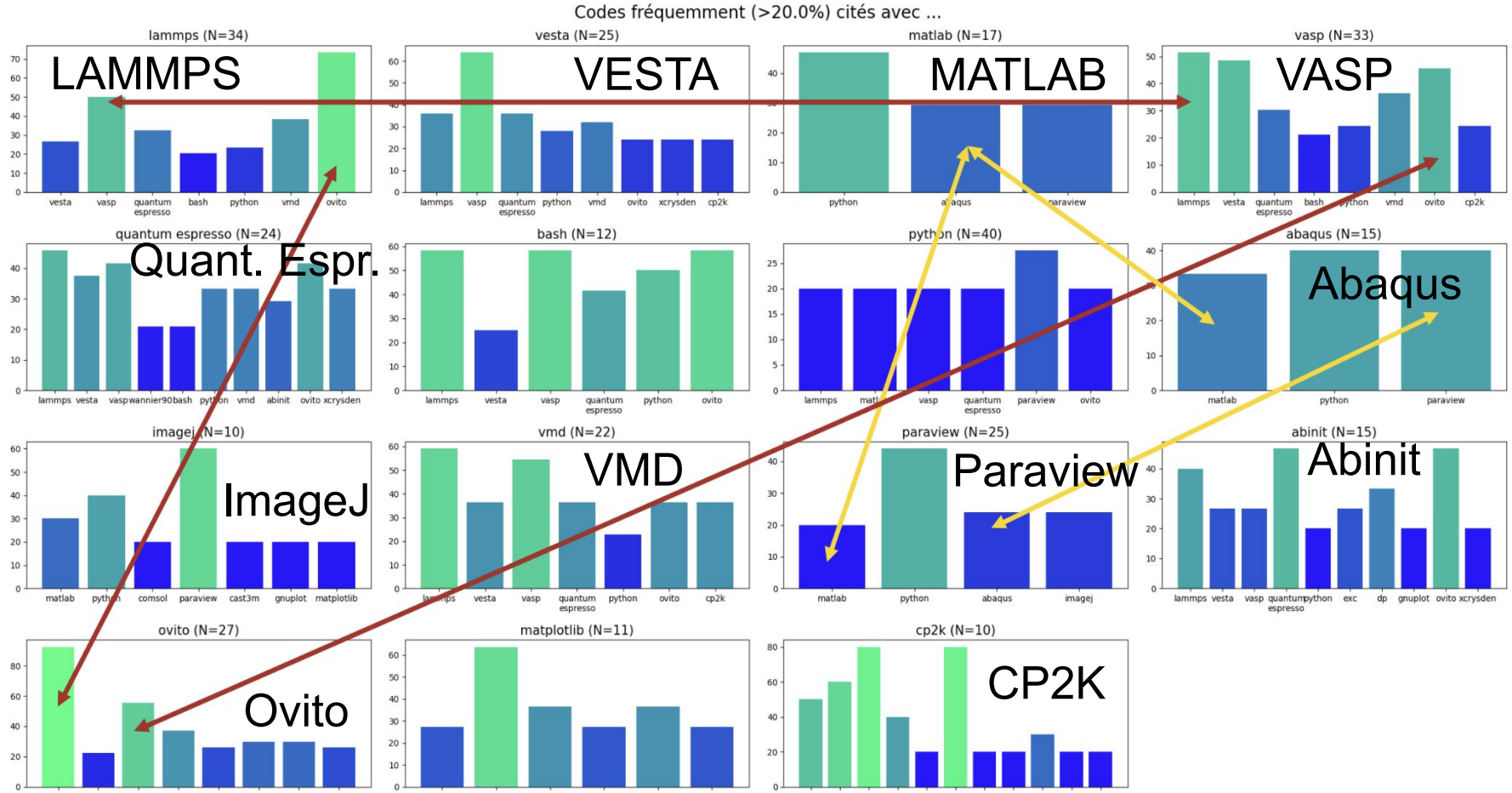
Materials Community Survey

LimeSurvey
limesurvey.org

Intelligence Artificielle en Sciences des Matériaux
GDR IAMAT
gdr-iamat.sciencesconf.org

- 1½ months - summer 2023
- 332 participations
- 111 complete answers

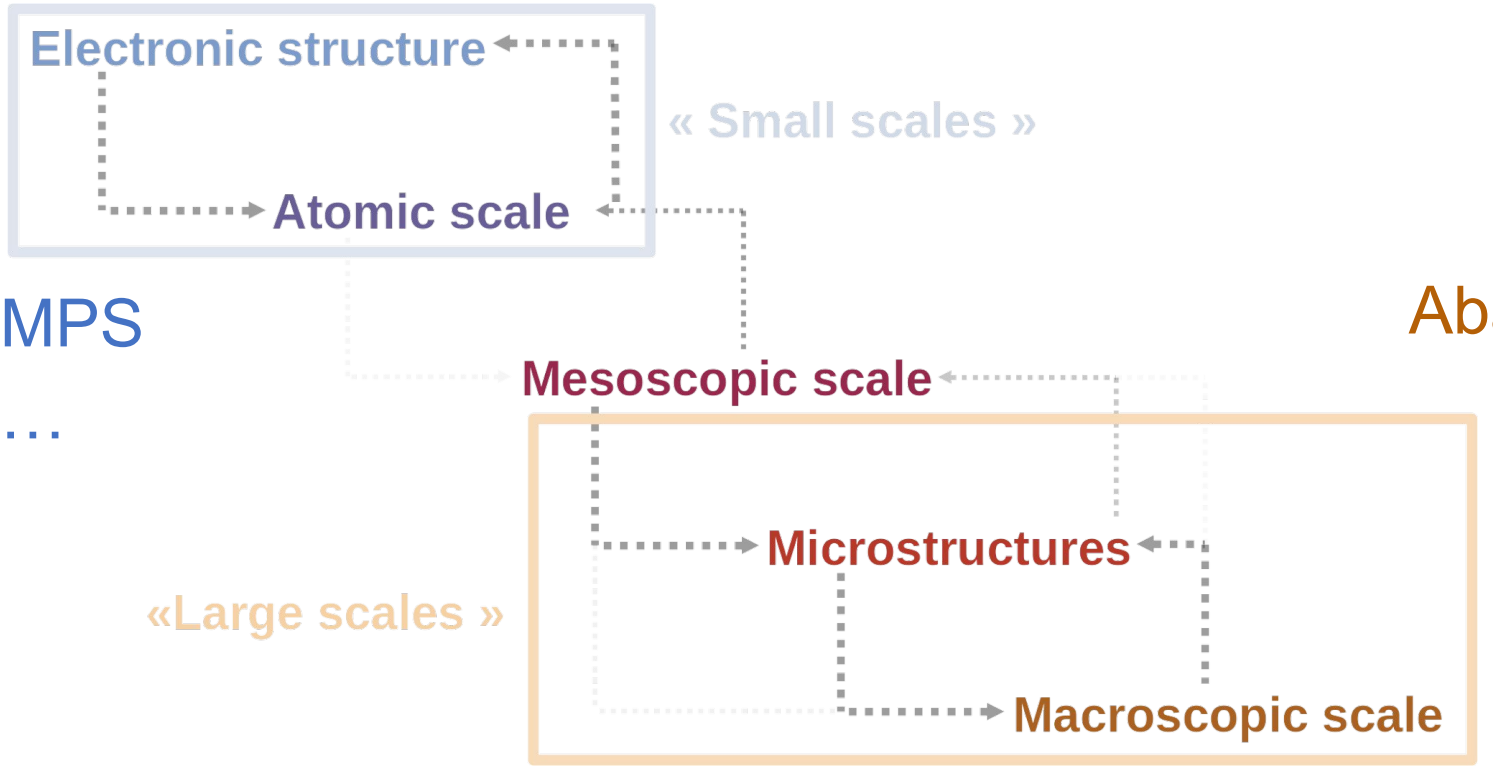


Materials Community Survey

LimeSurvey
limesurvey.org

Intelligence Artificielle en Sciences des Matériaux
GDR IAMAT
gdr-iamat.sciencesconf.org

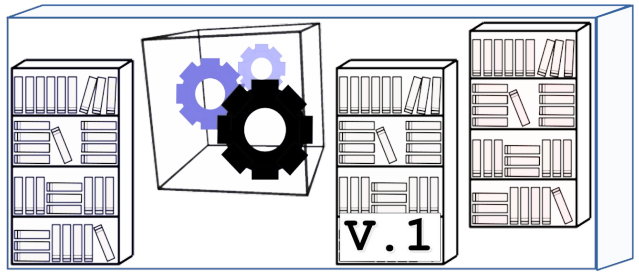
Two groups :

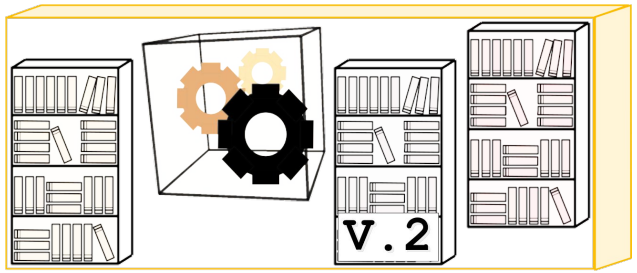


VASP+ LAMMPS
+ Ovito + …

Abaqus + Paraview
+ Matlab + …

Choice of the Tools





Containerization

as `docker`, …

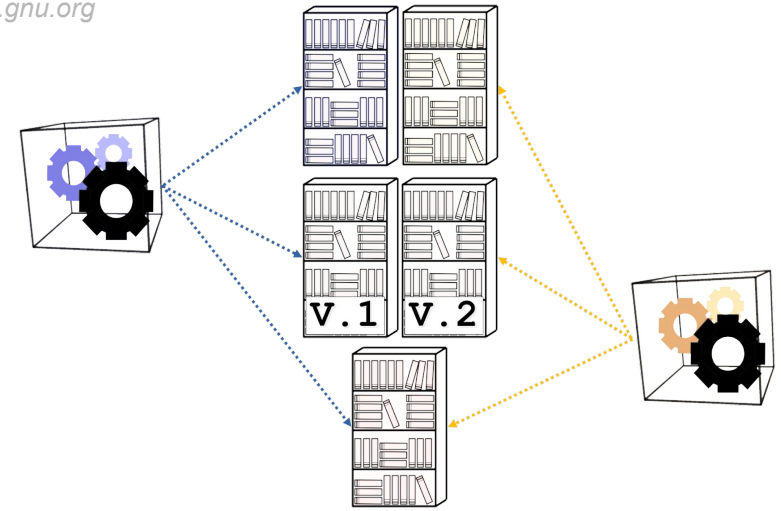
apptainer.org

Guix

guix.gnu.org

Package manager

as `apt`, `pip`, …



`guix pack <package>`

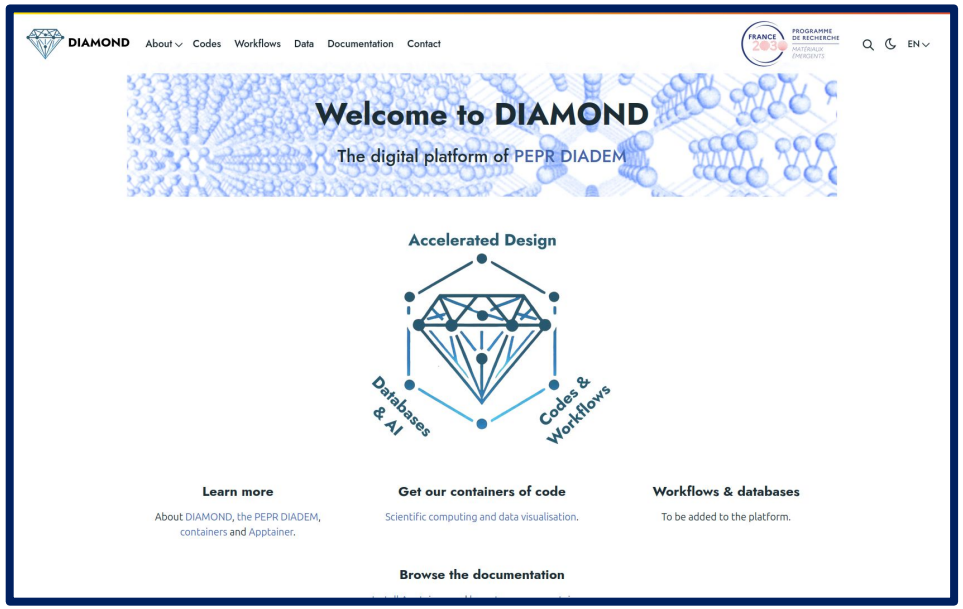
`apptainer pull <image>` ◀ - - - - - - - - - - - - - - - - `guix install <package>`

Website

Built with HUGO

https://gohugo.io/

The world's fastest framework for building websites



Hosted on Github

https://diamond-diadem.github.io/en/

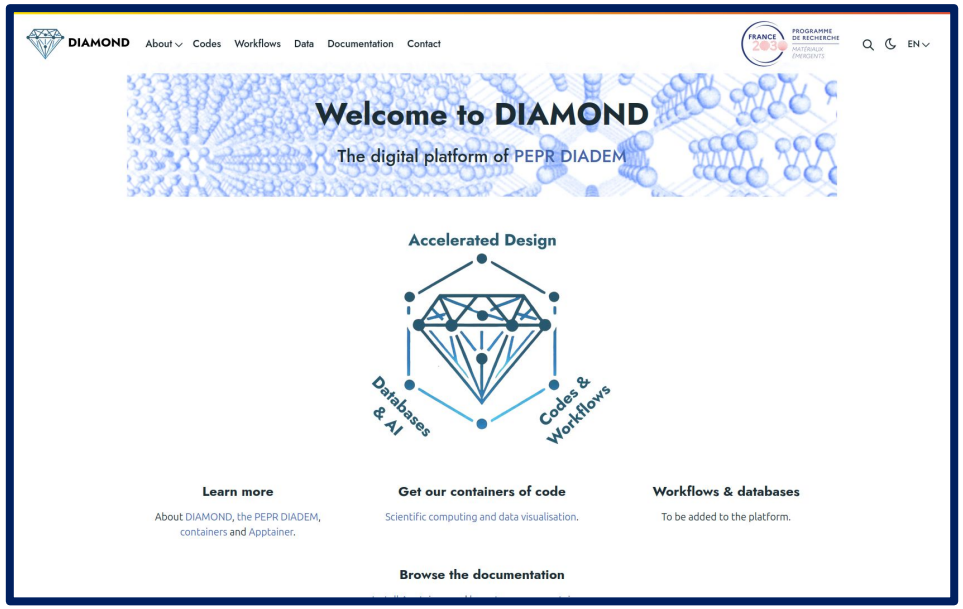
Doks theme, Thulite framework

https://getdoks.org/ https://thulite.io/

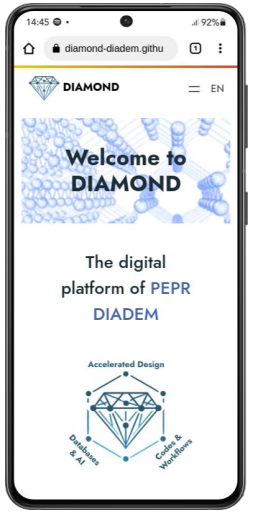
Strengths of this theme:

- ➔ light/dark mode
- ➔ efficient research tool
- ➔ language switcher
- ➔ dropdown menu

Website



Desktop 16:10



Galaxy S21

iPad Air

Desktop 9:16

Platform infrastructure

Why is it important?

The website is the **showcase** for DIAMOND and WP1, while the platform is the **final tool** used by users.

It should:

- make everything **accessible** to users
- help users to **contribute** to the project
- help users to **report** bugs or **request** new features
- make it easy to **manage** people working on the project
- **share resources** between engineers working on the project *(for today and tomorrow)*

Solution?

https://gricad-gitlab.univ-grenoble-alpes.fr/diamond

Everything is hosted on gricad-gitlab through:

- DIAMOND group *(public)*
- several subgroup, including Aiida and Apptainer *(public)*
- … and many projects *(public and private)*

Why choosing AiiDA ?

Covalent

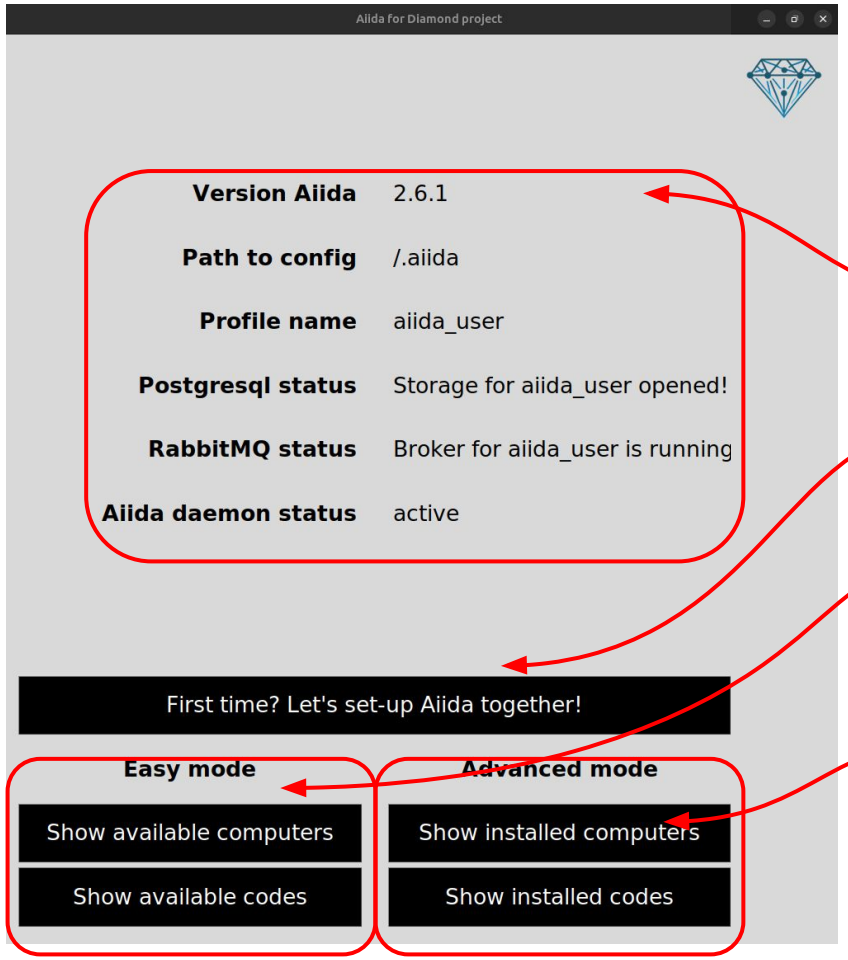
and many more …

Motivation :

- close connection with AiiDA developers at SIMaP
- significant list of existing plugins
- many schedulers implemented

} *In practice, AiiDA works with plugins (for codes) and schedulers (to use HPC facilities)*

Development of GUI for AiiDA Workflow Manager



The main objective is to make using AiiDA **as easy as possible**!

Multiple views for all users :

- information panel for current running version
- a beginner mode to guide the user through all steps
- an easy mode to install code or computer by just clicking on pre-made configurations
- an advanced mode to edit / delete codes or computers by just clicking on installed configurations

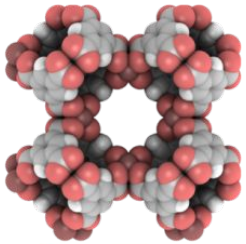
Development of workflows

Our engineers are currently involved in the development of a number of workflows, with the help of internal and external scientific specialists:

- **NUMODIS+LAMMPS workflow**, using **aiida-numodis** and **aiida-lammps** plugins.
- **AiiDA version of MOFLearning**
  - already functional for load balancing using **aiida-raspa**.
  - Works locally and at Jean Zay
- **Quantum Espresso workflow,** for MOF electronic structures
- **VASP workflow,** for post-processing molecular dynamics using geometry optimisation.
- **MLIP development workflow via n2p2** (by Akshay, in WP3)

Scientific specialists:

Laurent Dupuy



Arthur Hardiagon
François-Xavier Coudert

Ashna Jose
Roberta Poloni
Martin Uhrin

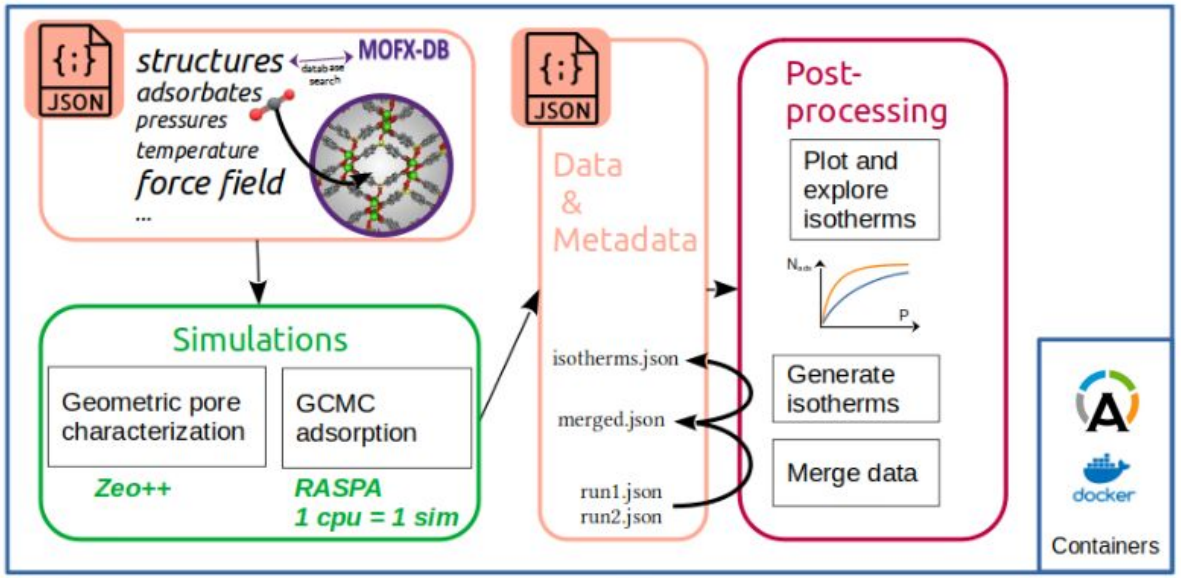
Noël Jakse

Arthur France-Lanord
Marco Saitta

Task 1.4 - Use case : MOF learning workflow

Workflow Python

- **Implementation and analysis:** A Hardiagon, FX Coudert
- **Technical support / containerization:** JPA Mendonca, D Bissuel



- Compute **adsorption properties** (Monte-Carlo)
- Materials : Metal-organic Frameworks from **CoRE-MOF 2019 database**
- **single-CPU** calculations

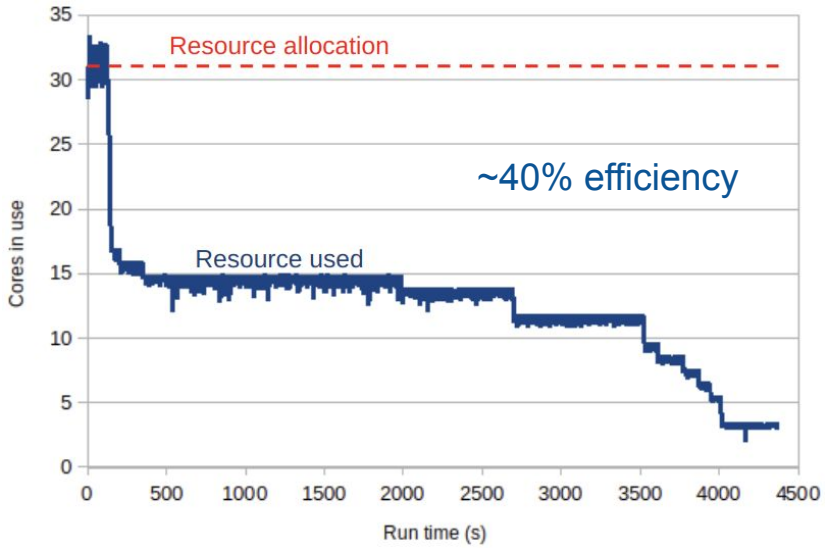
Functionalities

- JSON input/outputs
- GUI for input/output analysis
- **Container**
- Benchmark (Dahu, Gricad)

MOFs Learning : a data-based platform to accelerate functional MOF discovery
A Hardiagon, AY Ozturka, D Bissuel, JP Almeida de Mendonça, F-X Coudert
Oral presentation, 29/09 02/10 (2024)

Task 1.4 - Use case : MOF learning workflow

Benchmark (Gricad)



32 simulations on 32 CPUs
Parameters : **pressure, charge method, gas (N2,CO2)**

Issue :

- a Grand Canonical Monte Carlo simulation time is not easily predictable
- CPU efficiency is low

Solution :

- internal scheduler and queue system
- from another VASP workflow

⇨ Screening on large MOF databases (>40k) needs efficient solutions

Poster : A. Hardiagon

Task 1.4 - Use case : MOF learning workflow

Towards Complex Workflows for Database Screening

AiiDA

- **reproducibility**
- restart non-converged simulations
- full **control**
- existing **plugins**

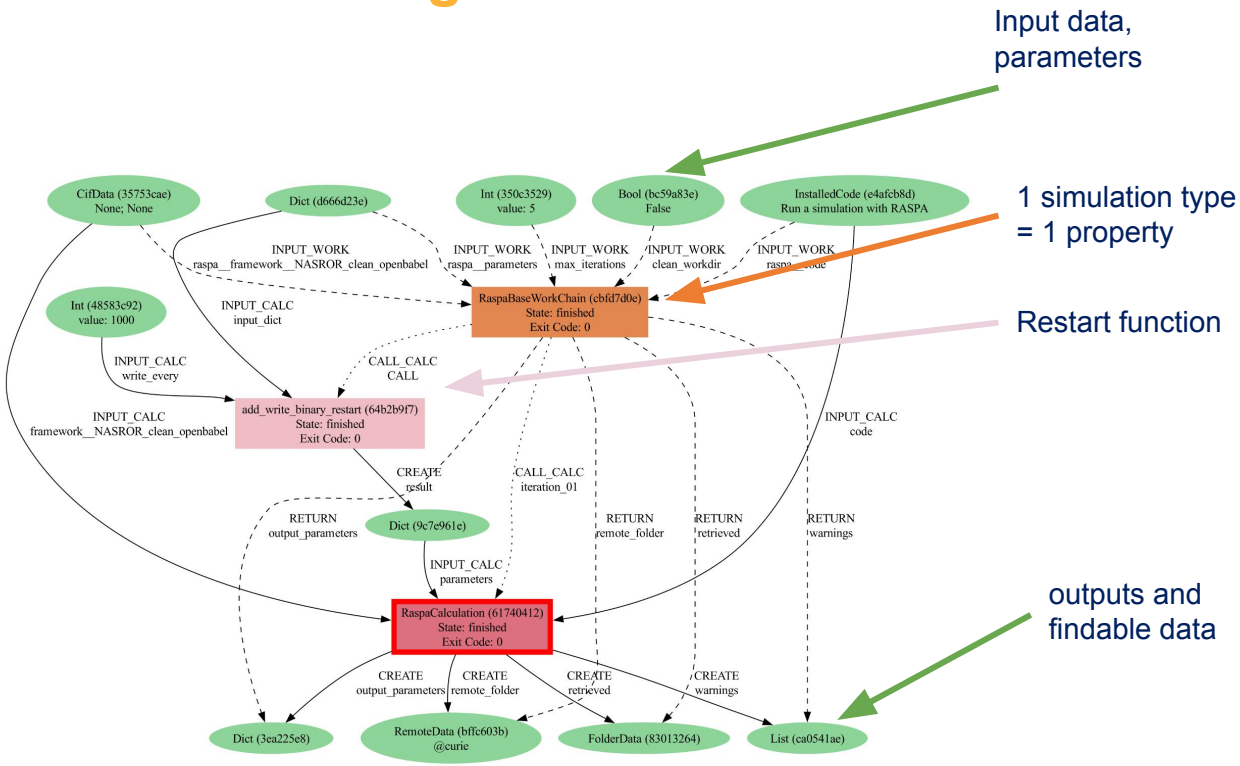
RASPA3

other thermodynamic properties :
- 2 gas adsorption
- heat of adsorption

LAMMPS

kinetic properties
self-diffusion of gas in porous media

⟹ Stable building blocks



Graph provenance from the plugin aiida-raspa

Other projects : spectra denoiser (LIBELUL)

LIBELUL: LIBS for high-throughput elemental analysis

https://www.pepr-diadem.fr/projet/libelul-en/

- DIADEM **targeted project**
- LIBS: Laser Induced Breakdown Spectroscopy
  - analyzing the **fluorescence emission spectrum** of the **plasma** induced by the **ablation of the material** to be analyzed by a **laser pulse.**
- coupled with **RAMAN** and Luminescence spectroscopy

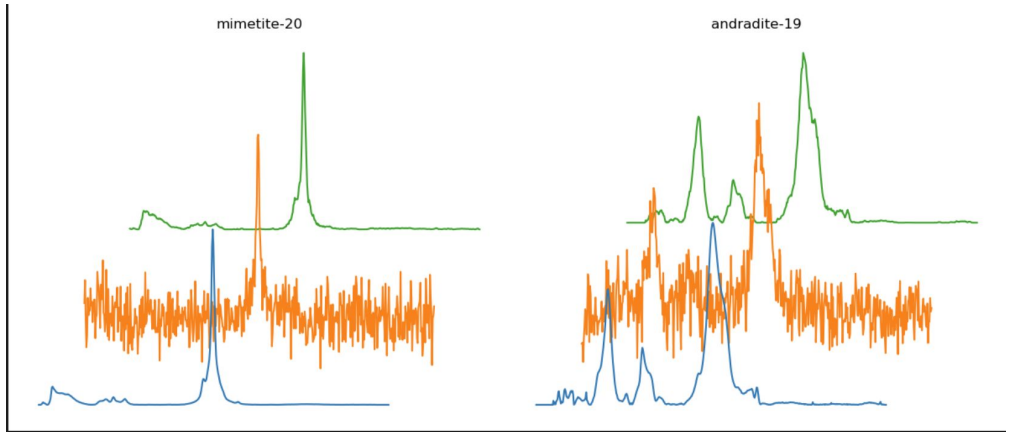
Proposal to develop a tool to denoise RAMAN spectra

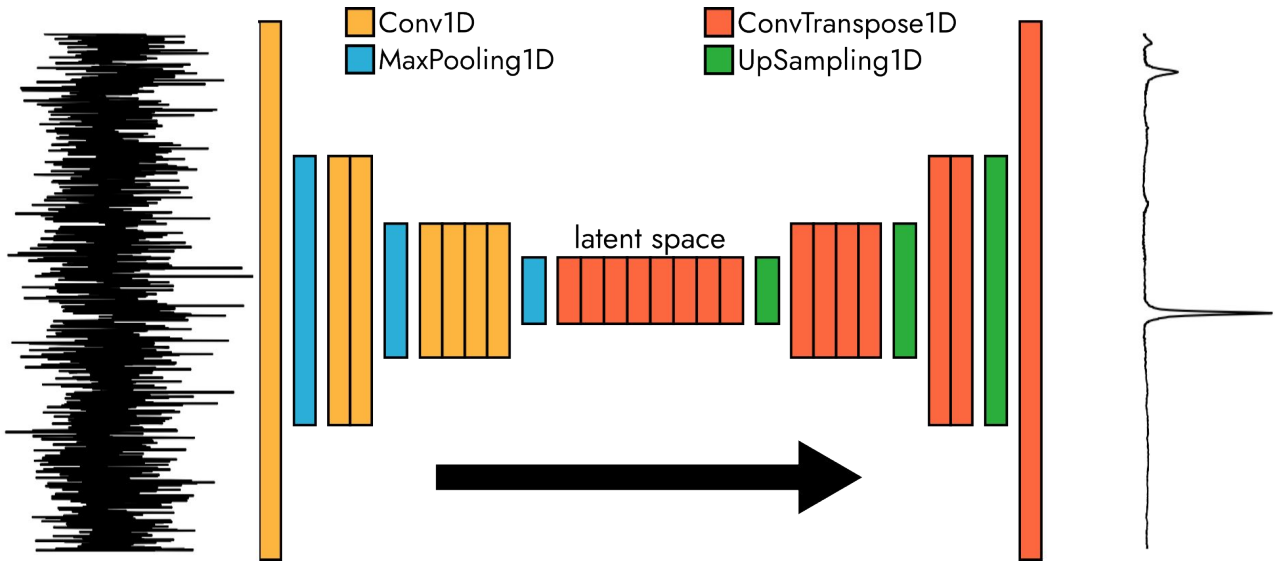
- Objective: **decrease acquisition time** (from ~ 1 minute to ~ 0.1 second)
- Noisy spectra, which require **denoising**

Other projects : spectra denoiser (LIBELUL)

Development of a denoising auto-encoder (DAE)

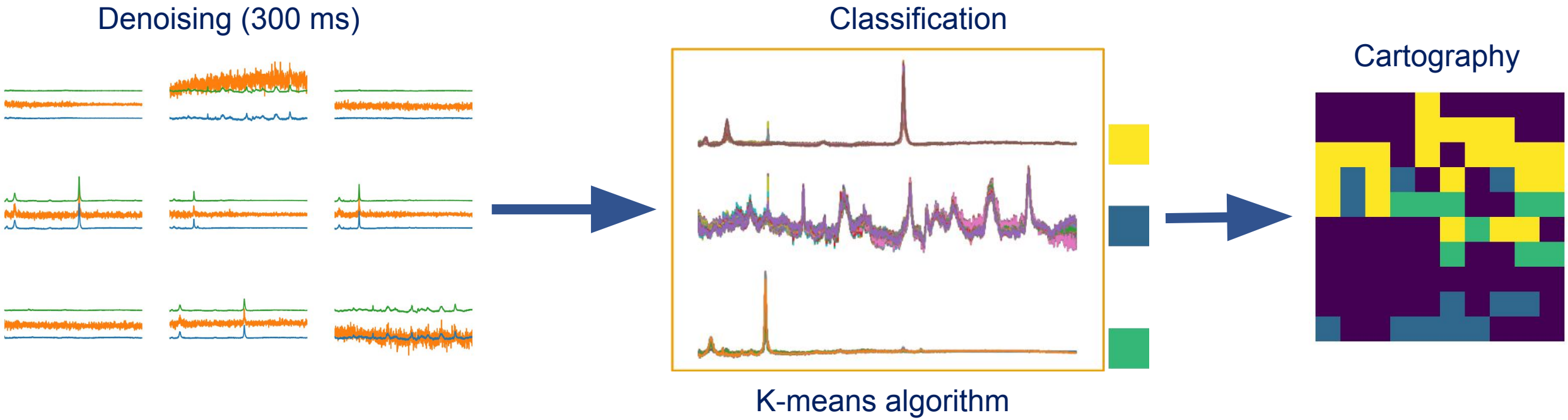
- Encode and compress the initial spectrum in a latent space of reduced dimensionality (Keras+pytorch)
- Decode the encoded features into a clean spectrum (Keras+pytorch)





Other projects : spectra denoiser (LIBELUL)

First step towards automated mapping



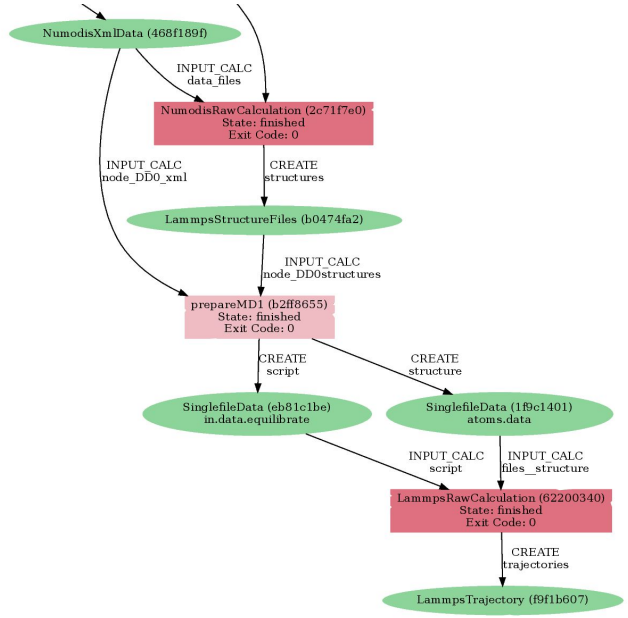
Workflow example: NUMODIS + LAMMPS

Test case for workflow automation

- Atomistically-informed simulation of dislocation dynamics.
- Run from an AiiDA container.

Benefits of the automation using AiiDA as a Workflow manager

- AiiDA's provenance graph keeps track of the data origins; Reproducibility.
- Containerized solution to share not just the data but also the workflow for reproduction.
- Automation allows generalization, to change initial conditions, materials, etc…
- Reduces the risk of mistakes when changing initial parameters.



example of provenance graph

Conclusion

The basis of the infrastructure is setup and shows a good robustness

- Containerization and package solutions as well as Workflow solutions

Tested successfully on several use cases for workflows

- mostly at small scales (atomic- and meso-scale)

Seeking some collaborations and ideas of workflows including also ML/AI to setup from other DIADEM projects

- Larger scales and especially materials processing could interesting to include in the platform

Contact us on diamond website or by email