

Description

AiiDALab is a web platform that enables computational scientists to package scientific workflows, computational environments and associated graphical user interfaces so they can be shared with their collaborators and peers. Computational workflows can be bundled together with user-friendly graphical interfaces and made available through the AiiDALab app store. It lowers the entry barrier for setting up a computational research software environment and significantly simplifies the execution of complex scientific workflows.

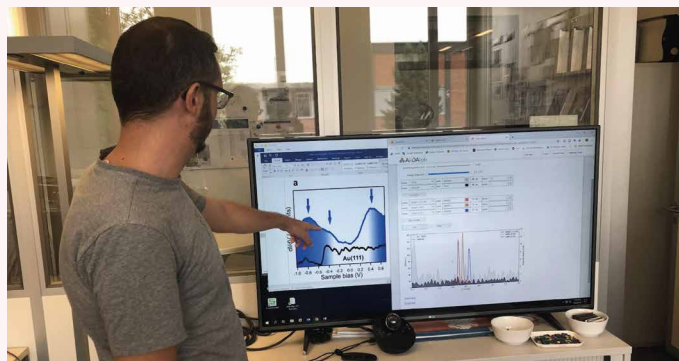
Key Features

- ◆ A cloud platform where you launch and monitor AiiDA workflows, and analyze the results from browser.
- ◆ Dedicated applications with intuitive graphical user interfaces.
- ◆ Sharing of apps and workflows via the AiiDALab App Store.
- ◆ Fast development of new apps as Jupyter notebooks.
- ◆ Open technologies throughout - host your own AiiDALab!

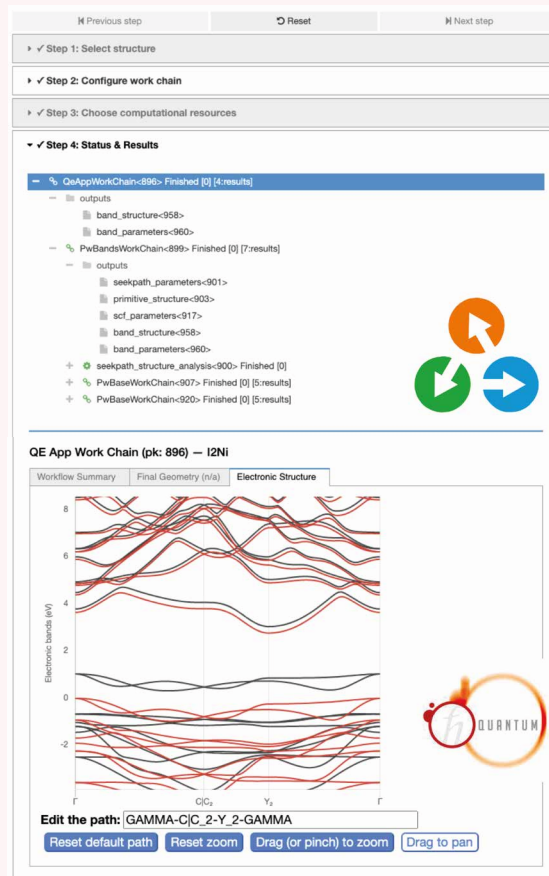
Technologies

- ◆ AiiDA as workflow manager to orchestrate workflows and retain data provenance.
- ◆ Jupyter web technology as graphical interface to develop and interact with App.
- ◆ The AiiDALab environment is distributed as a Docker container image and a virtual disk image as part of the Quantum Mobile virtual machine.
- ◆ The distribution of applications via the AiiDALab app store is facilitated by git and GitHub.

Practical use



The use of AiiDALab accelerates enormously the interaction between experiments and simulations at Empa, and thus time to discovery.



Use of the AiiDALab QE app to run DFT simulation on Quantum ESPRESSO to compute the band structure of two-dimensional magnetic Van der Waals NiI₂. Open the QE app directly in the browser and launch the calculation without the need for locally installed codes.

App Registry

Available AiiDALab apps are listed in a central "AiiDALab registry". Once an app is added to the registry, it is automatically listed in the AiiDALab App Store of every AiiDALab user. Each entry in the registry contains the minimum information about an app: its name, a link to its Git repository, a link to a metadata file, and a list of categories it falls within. Such an infrastructure provides AiiDALab application developers with an efficient way to share their scientific expertise and knowledge (encoded into the application and the workflows) with the rest of the community, while maintaining full ownership and control on the development of the apps.

Total number of apps: 9

Available apps



Quantum ESPRESSO

Current state: development

Perform Quantum ESPRESSO calculations

[Show app details](#)



SSSP toolbox

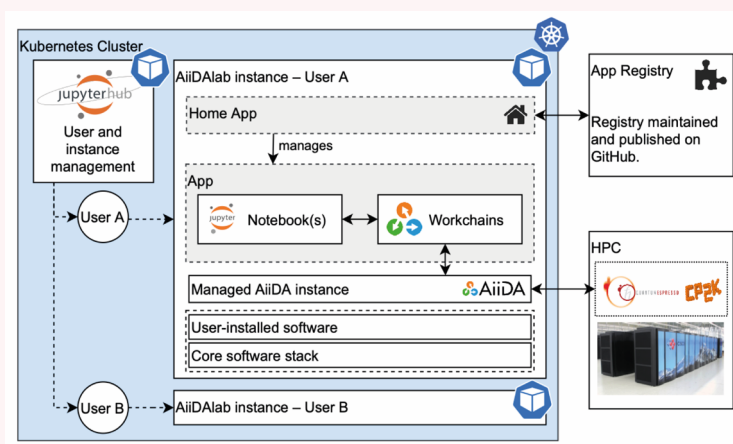
Current state: development

AiiDALab app to run pseudopotential verification.

[Show app details](#)

Architecture

Users are authorized through JupyterHub (which performs the authentication through an external identity provider service) and assigned to a specific personalized AiiDALab instance – a Docker container with an AiiDA instance and a Jupyter-based environment to manage AiiDALab apps. The apps contain Jupyter-based user interfaces and AiiDA workflows, which communicate with the AiiDA instance. New apps can be installed through the App store app, which is a user interface to the AiiDALab application registry.



Contact & Support



Website



Github



App Store



AiiDALab docs

References

■ A. V. Yakutovich et al., *Comp. Mat. Sci.* **188**, 110165 (2021) DOI - 10.1016/j.commatsci.2020.110165