

**PSI**

Center for Scientific Computing,  
Theory and Data

# Executing Complex Scientific Workflows in the Browser

**AiiDAlab Quantum ESPRESSO App**

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## Domain experts

- Advanced experimental techniques
- Specific materials and their applications: catalysis, battery materials

Not trained in programming or computational skills for a computational code.

Need a tool that enables domain experts to implement DFT pipelines and learn how and when to apply DFT calculations to their research.

## Computational material scientist

- Advanced DFT theory and approaches
- Computational codes.
- Programming skills

Lack understanding regarding the real-world application without reading the domain-specific literature

# Bring the first-principle tools to larger communities



Broadly available simulation codes and workflows.



Barrier



Domain experts  
(experimentalists)

Software Installation  
and Configuration  
Input File Preparation  
Parameter Tuning  
Interpreting Results  
Computational Resources  
Validation and Benchmarking



Empa

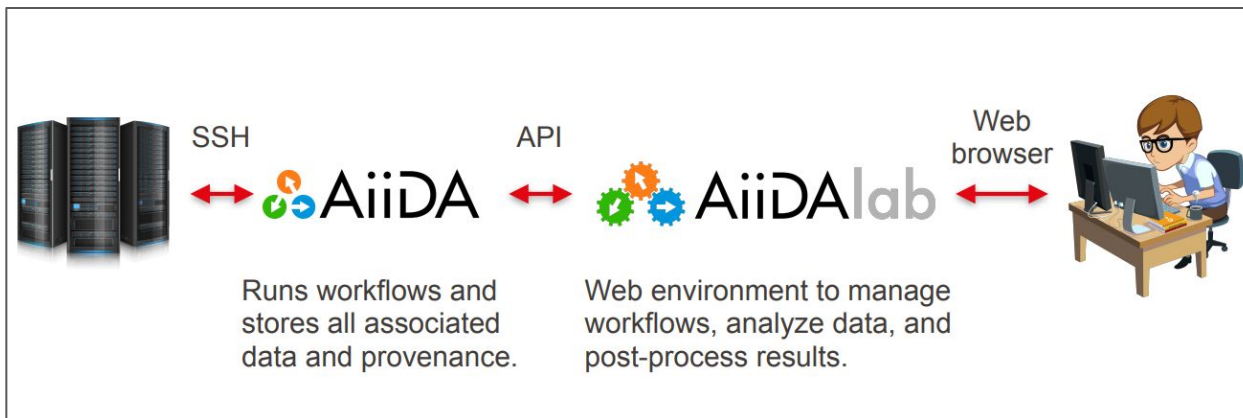
Materials Science and Technology



# Automated, reliable, "turn-key" simulations tool

Quantum ESPRESSO (QE) app is an AiiDA lab web-based graphical user interface allowing users to conduct first-principle calculations on the web browser directly without writing any code.

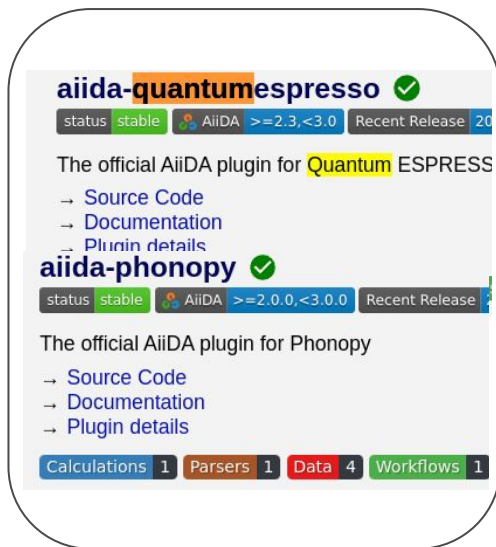
- Automated
- Reliable
- Intuitive user interface
- Easy to share and maintain



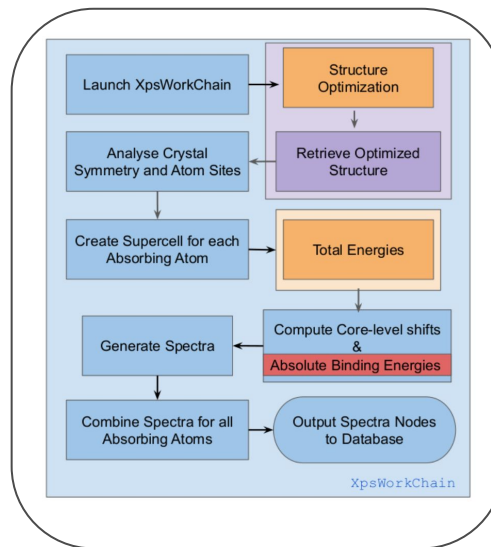
FAIR (Findable, Accessible, Interoperable, and Reusable) data.

FAIR access to simulations, workflows, and analysis tools

AiiDA's workflows implemented in the AiiDA Quantum ESPRESSO and others plugins.



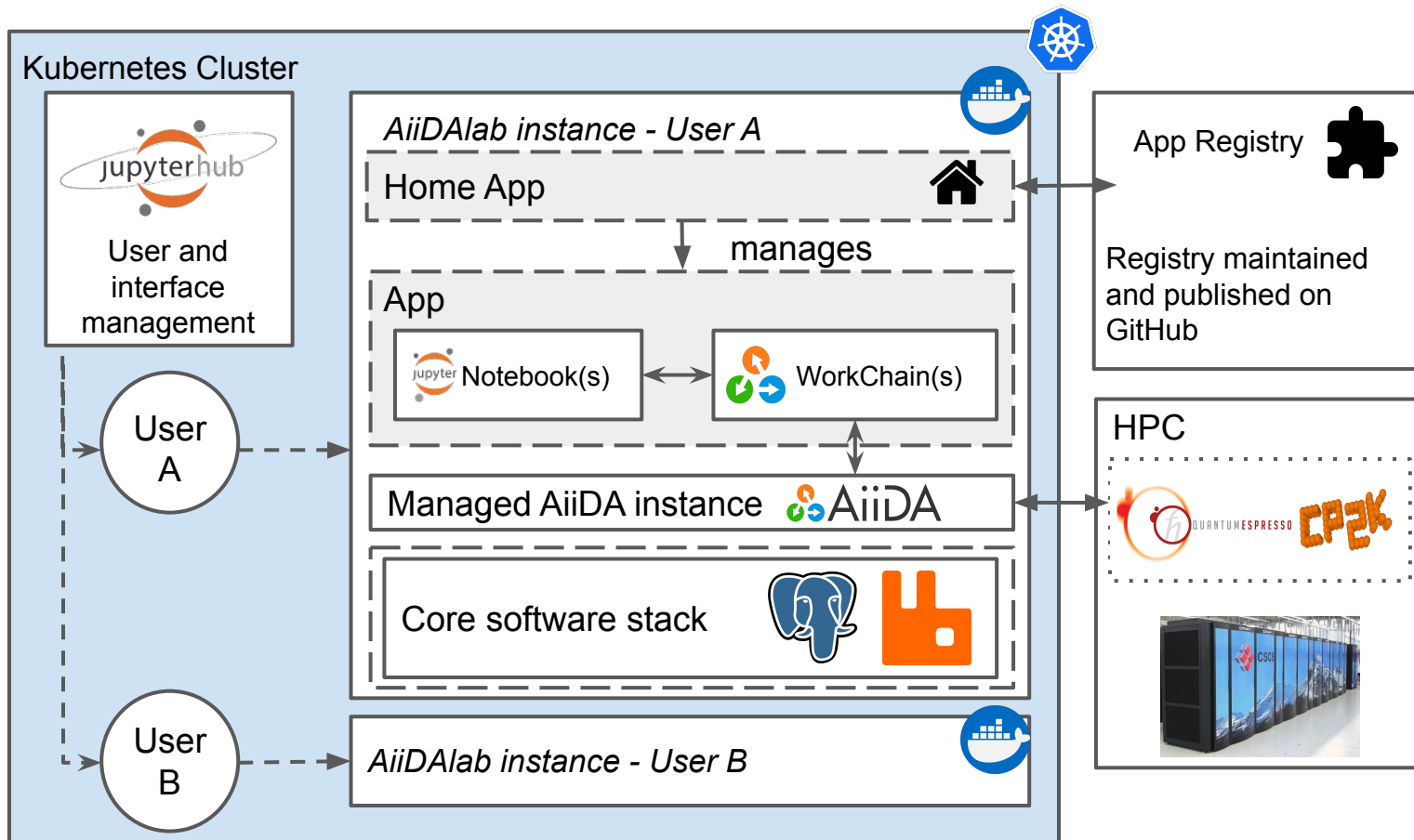
The screenshot shows two AiiDA plugin pages. The top page is for 'aiida-quantumesspresso', which is marked as 'stable' and compatible with AiiDA versions '>=2.3, <3.0'. It is described as 'The official AiiDA plugin for Quantum ESPRESSO' and includes links for Source Code, Documentation, and Plugin details. The bottom page is for 'aiida-phonopy', also marked as 'stable' and compatible with AiiDA versions '>=2.0.0, <3.0.0'. It is described as 'The official AiiDA plugin for Phonopy' and includes links for Source Code, Documentation, and Plugin details. At the bottom of the Phonopy page, there are statistics: Calculations 1, Parsers 1, Data 4, and Workflows 1.



XPS workflow



# Architecture





# How to access?

- Docker image: [aiidalab/qe:latest](https://aiidalab.org/docker/qe:latest), with pre-built environments, e.g., pseudopotentials, code setup.

Single User



1-50 Users



100-1000+ Users



[Documentation](#)



[GitHub](#)



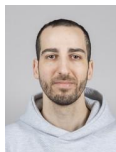
- We also maintain a few official cloud-backed deployments  
<https://aiidalab.psi.ch/>  
<https://demo.aiidalab.io/>



# Acknowledgements - AiiDA, AiiDALab, Materials Cloud



The current AiiDA, AiiDALab  
and Materials Cloud teams



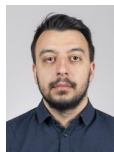
Edan  
Bainglass  
(PSI)



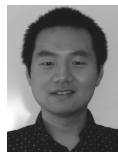
Roberto  
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Bercx  
(EPFL)



Miki  
Bonacci  
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P. Huber  
(Microsoft)



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Chris  
Sewell  
(EPFL)



Leopold  
Talirz  
(Microsoft)



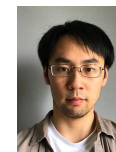
Joost  
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(ETHZ, CSCS)



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(EPFL)



Aliaksandr  
Yakutovich  
(Empa)



Jusong  
Yu  
(EPFL)



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Guerrero  
(Empa)

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- Dr. Prezzi's group on the XPS and XAS plugins

