



AiiDA lab - an ecosystem to develop, execute and share scientific workflows

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Outline

- Motivation & intended user base (5 min)
- AiiDA lab interface overview (5 min)
- Examples of daily scientific work with AiiDA lab (12 min)
- Future plans & conclusion (3 min)

Motivation

Computational Materials Science Challenges

High-Throughput

Reproducibility

Open Data

Knowledge Transfer

- How to transfer your insights & expertise, e.g.
 - reporting data sets to an experimental group
 - providing a workflow for your code to a collaborator/company
 - ...
- PDF report via email?
- Give a presentation?
- ...?

Source: quote.ucsd.edu



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User base

User	Skills	Goals	Solution
Computational Scientist	Knows Unix, bash, python	• run high-throughput calculations • write complex workflows • develop AiiDA plugins	AiiDA on the laptop
Experimental Scientist	Doesn't know Unix, bash, python	• run pre-defined workflows • analyze results	AiiDA lab in the cloud
Student (tutorial/lecture)	some familiarity with Unix, bash, python	• learn how to use AiiDA • learn how to use ab-initio codes • take materials home	Quantum Mobile on the laptop

AiiDA vs AiiDA lab



Features:

- Can run complex workflows
- Stores computed data locally
- Stores the data provenance
- Python or command line interface
- Integrated with AiiDA
- User-friendly web interface (Jupyter notebooks & widgets)
- Easy application development (directly in Python)
- App Store for sharing your applications

AiiDA lab interface overview



File Manager

Browse files



Terminal

Linux terminal



Tasks

Manage running apps



App Store

Install apps
Update apps
Uninstall apps



Help

Know more about AiiDA lab

AiiDA lab application

App name

▼ AiiDA Cockpit

- Daemon Status
- Workflows
- REST API
- Graph Browser
- Delete nodes

Notebooks

Update Info

✓ Latest Version

Move up/down

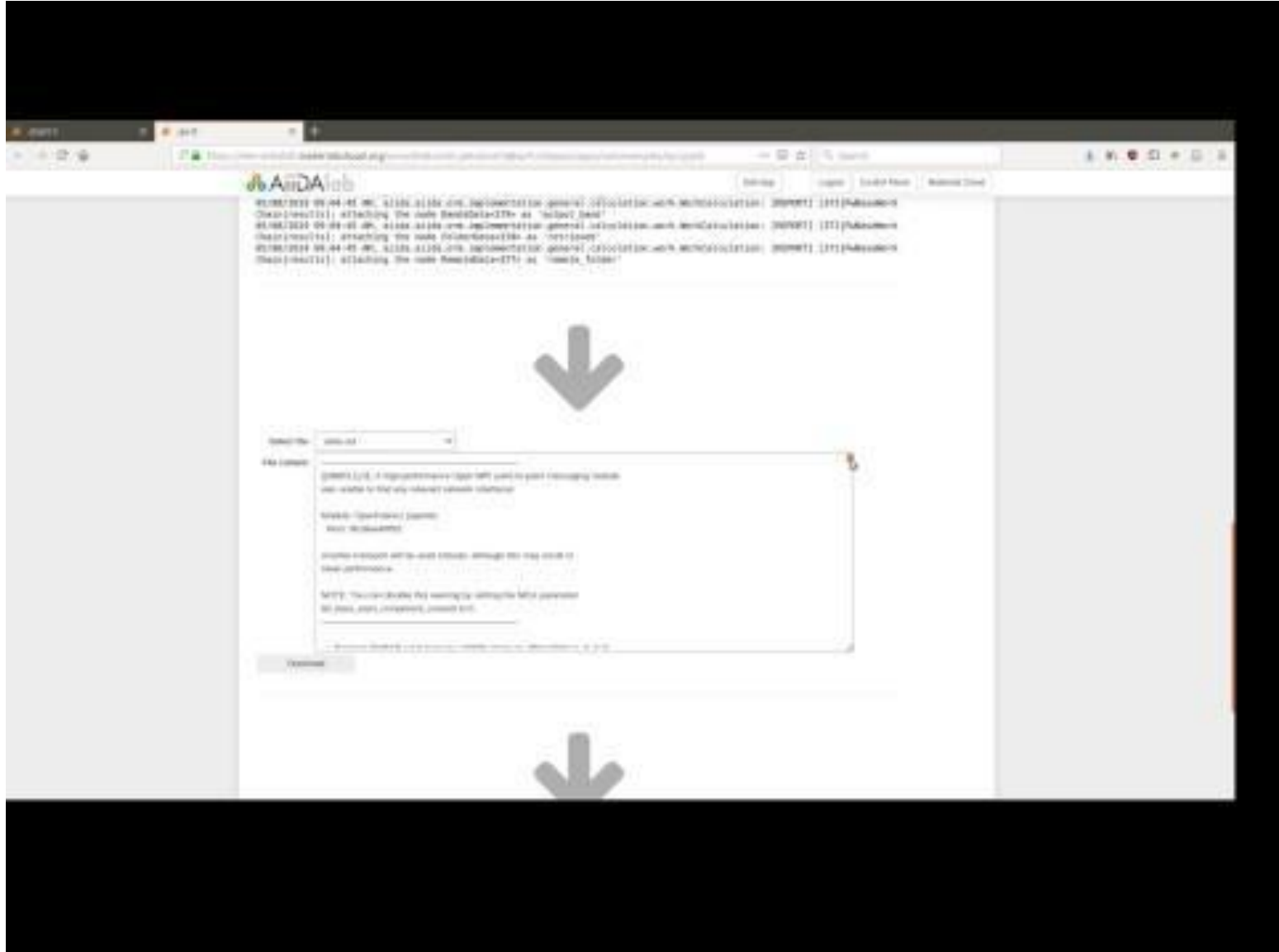


Install, uninstall,
update, select version

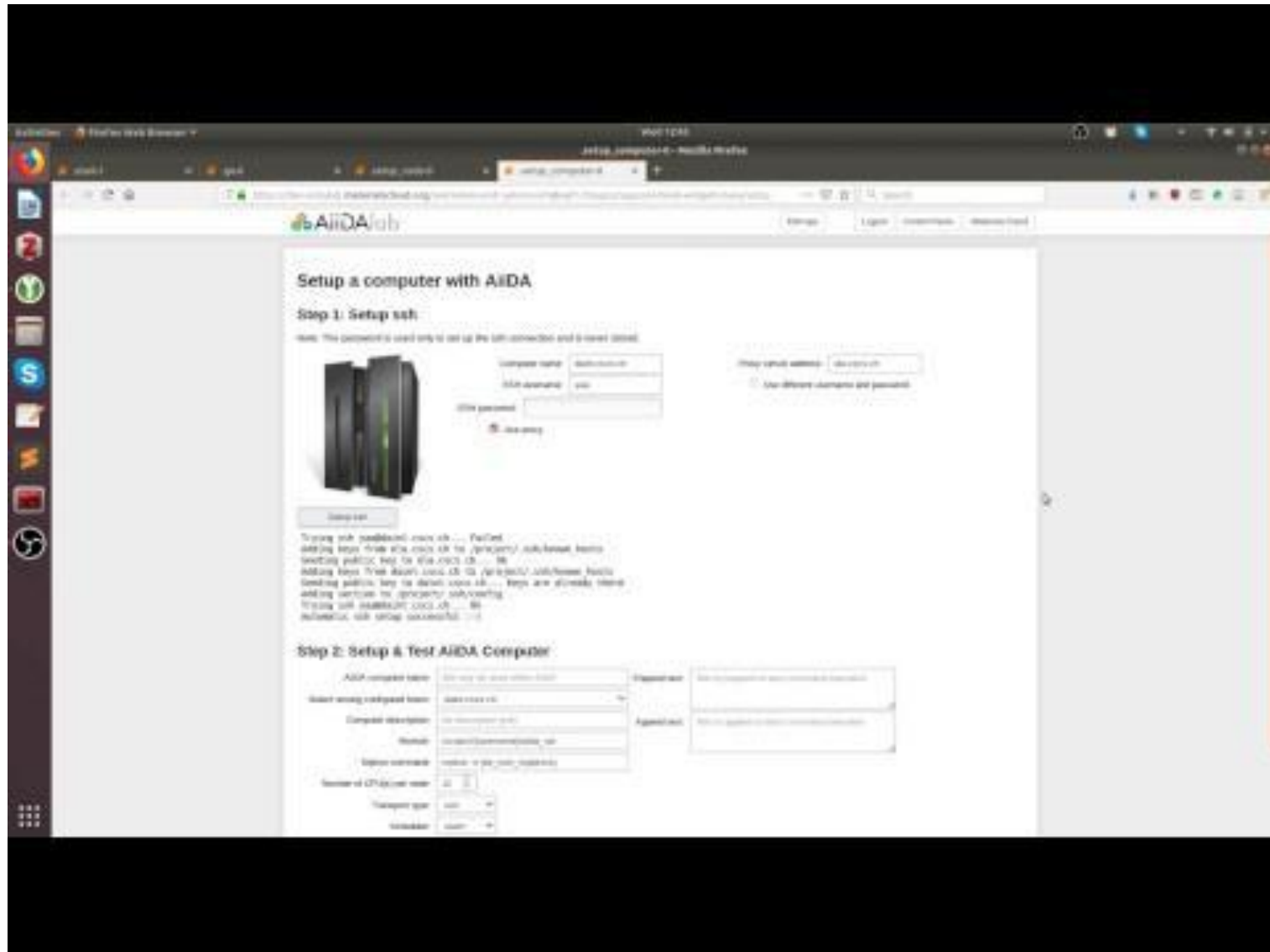
Manage App

Git URL

AiiDA lab demo application



Setup new code and computer



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Example from Empa

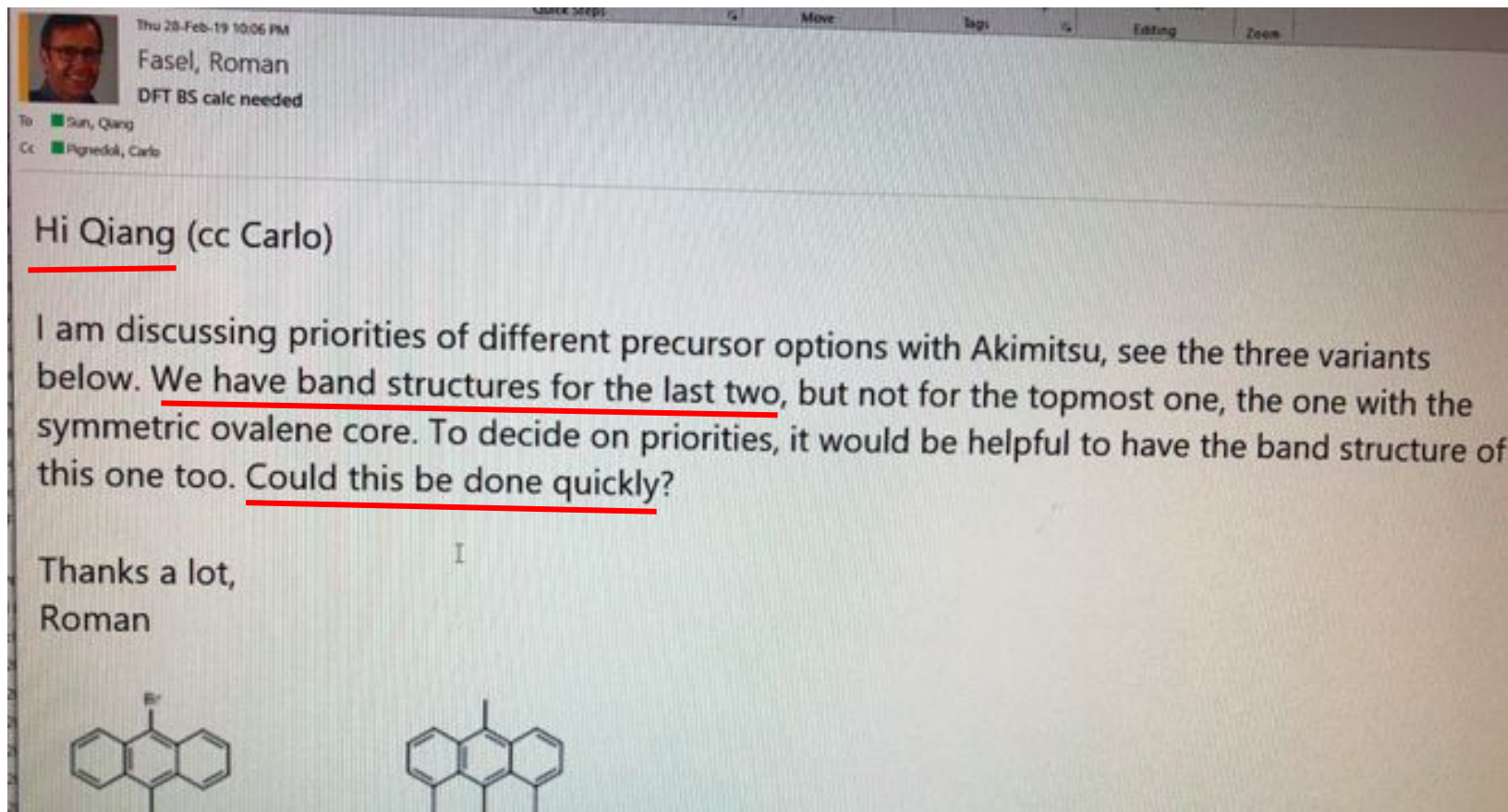
Before AiiDA lab the typical questions from experimental scientists would be:

- Some while ago* we discussed ribbons A, B, C. Did you compute the band structure?
- Does it take long to have the band structure of ...?

* can be more than 1 year ago

Example from Empa

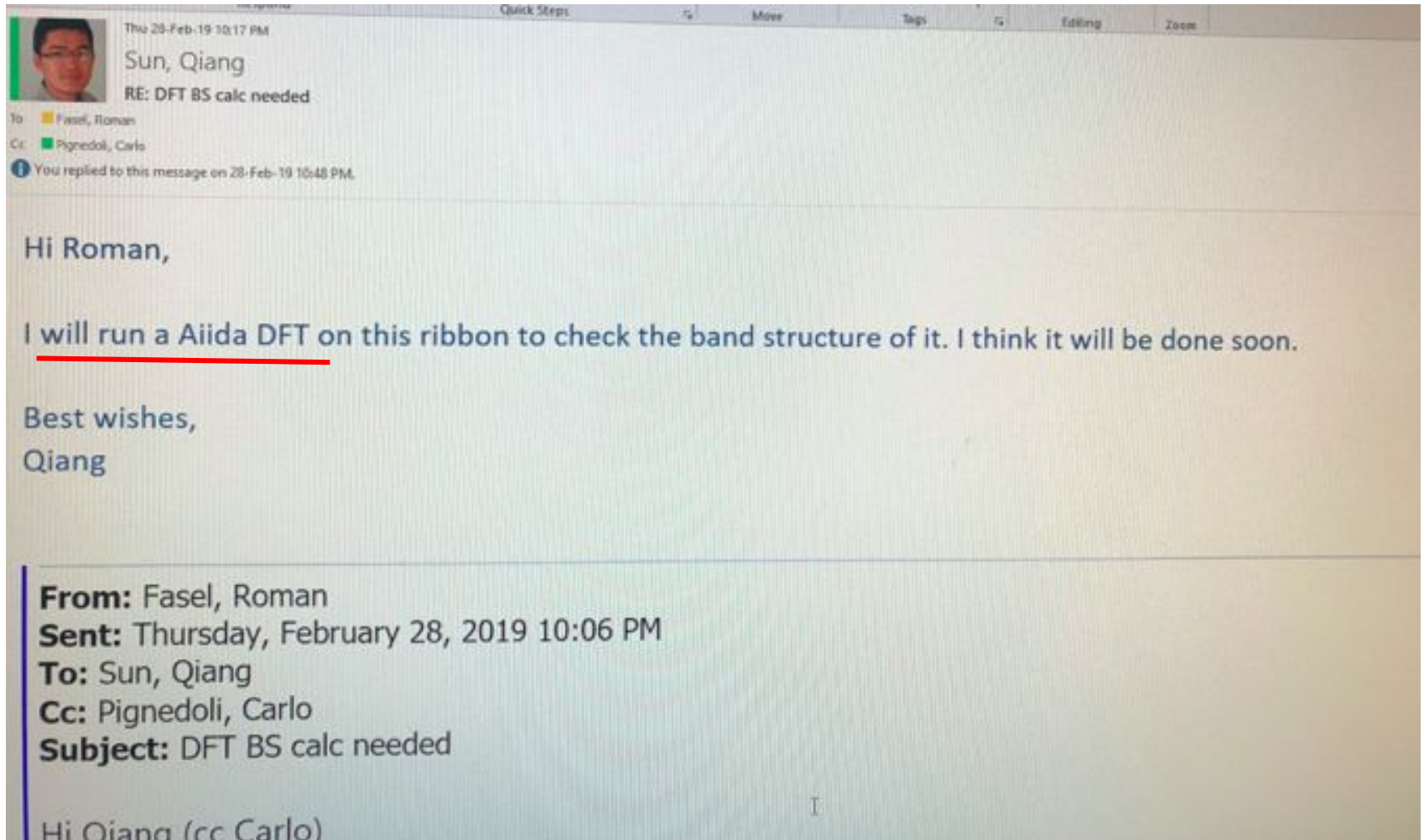
... now



- Request to run calculations directly addressed to an Exp Phd
- Status of available calculations known
- Implicitly expecting this will be fast

Example from Empa

... now



- no support needed

Make your own app:



Help

Make your own app

Leopold Talirz edited this page on Feb 12 · 4 revisions

Edit

New Page

Variant A: Quickstart using the AiiDA lab application cutter

Open the terminal from the AiiDA lab home page. On the terminal type:

```
$ cd apps
$ cookiecutter https://github.com/aiidalab/aiidalab-app-cutter.git
app_name [template]:
...
```

After answering the questions asked by the app cutter, you will find a new folder inside `apps` that contains the basic structure of the app. In order to see the rendered version of your app, simply open (or reload) the home page.

▼ Pages 4

Find a Page...

[Home](#)

[Intro](#)

[Make your own app](#)

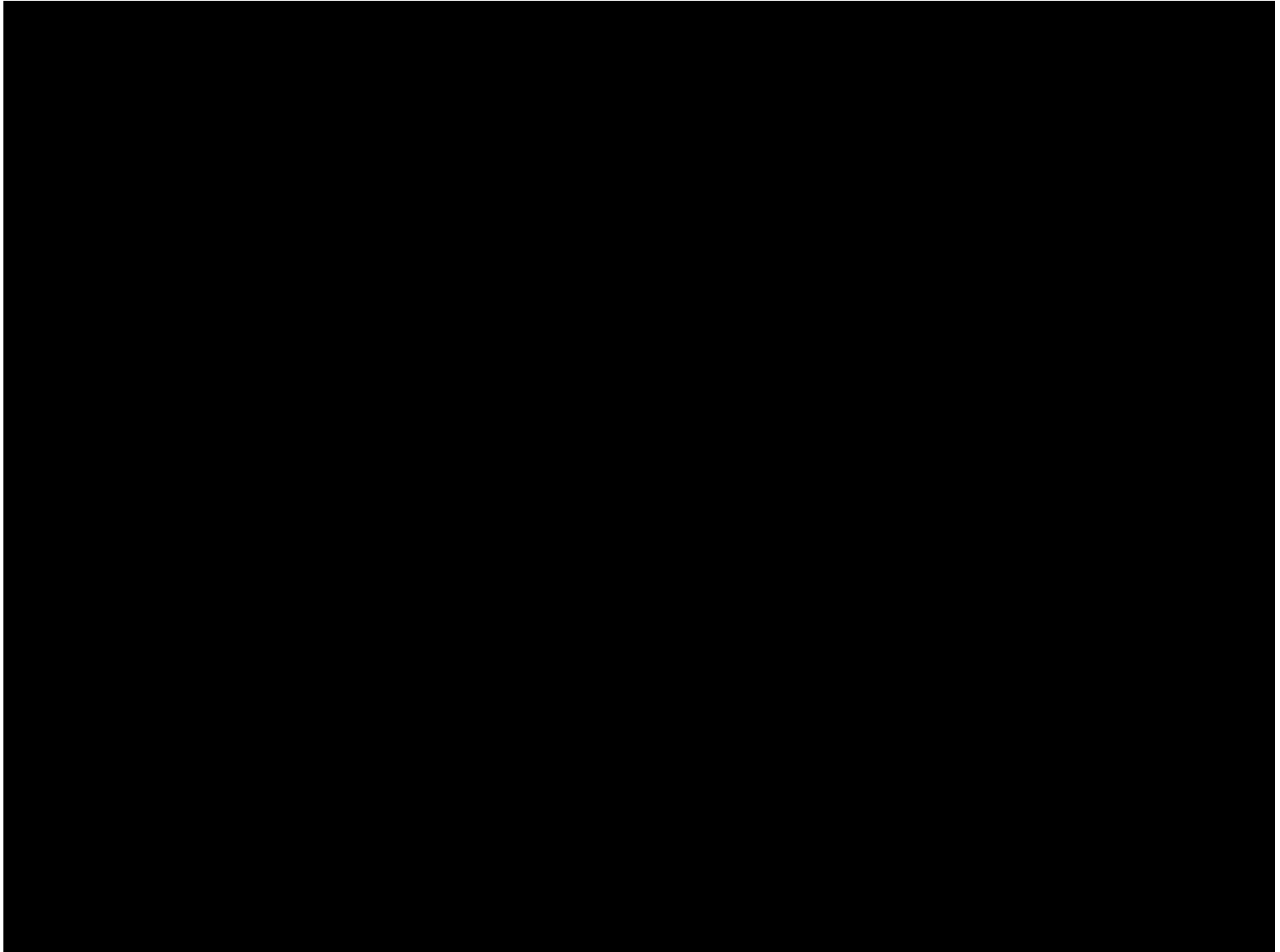
[Working with AiiDA lab](#)

+ Add a custom sidebar

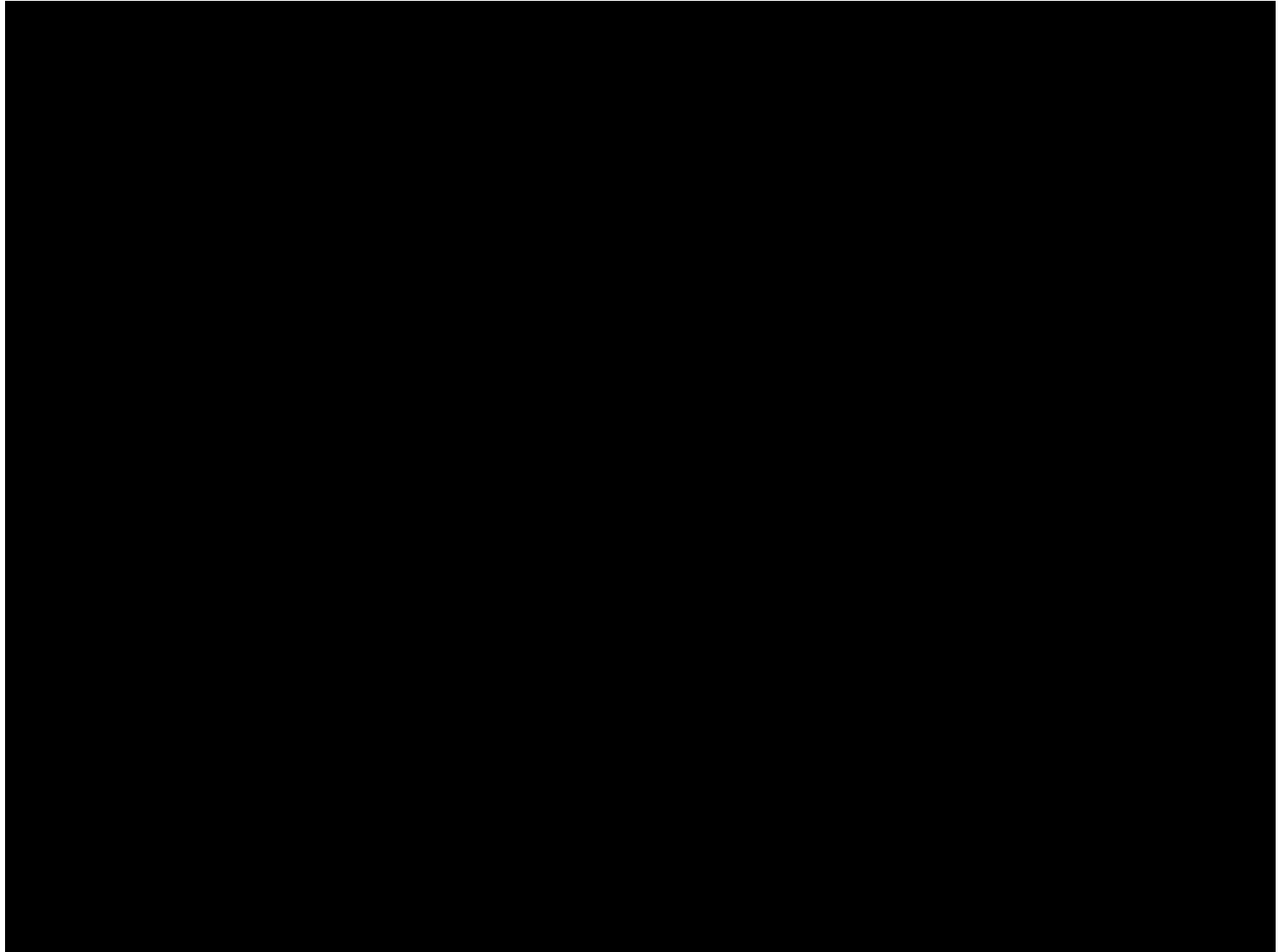
App is a folder that contains the following files:

- metadata (name, authors, description)
- startup file (start.py or start.md)
- collection of Jupyter notebooks

Make your own app



AiiDA lab App Store



Quantum Mobile Virtual Machine

Terminal window output:

```
(aiida) max@qmobile: ~/codes$ verdi code list
# List of configured codes:
# (use 'verdi code show CODEID' to see the details)
* pk 1 - yambo-4.2.0@localhost
* pk 2 - p2y-4.2.0@localhost
* pk 3 - fleur-0.27-fleur@localhost
* pk 4 - fleur-0.27-mpgen@localhost
* pk 5 - siesta-4.0.1@localhost
* pk 6 - cp2k-5.1@localhost
(aiida) max@qmobile: ~/codes$ verdi calculation list -a
# Last daemon state_updater check: 0h:00m:05s ago (at 15:09:17 on 2017-11-20)
```

PK	Creation	State	Sched. state	Computer	Type
175	3h ago	FAILED	DONE	localhost	siesta.
179	3h ago	FINISHED	DONE	localhost	fleur.i
195	3h ago	FAILED	DONE	localhost	siesta.
208	3h ago	FINISHED	DONE	localhost	siesta.
221	11m ago	FINISHED	DONE	localhost	fleur.i
228	11m ago	FINISHED	DONE	localhost	fleur.f

Total results: 6

(aiida) max@qmobile: ~/codes\$

3D visualization window (jmol) showing a crystal structure with parameters:

```
P 1 [P 1]
a=3.188Å
b=3.188Å
c=23.155Å
α=90.0°
β=90.0°
γ=120.0°
```

Quantum Mobile
MARVEL
MAX

- Ubuntu 18.04 LTS
- AiiDA, AiiDA lab
- QE, Siesta, fleur, yambo, CP2K, ... + AiiDA plugins
- Visualization tools (xcrysden, ...)
- used in tutorials & lectures at EPFL, ETH, ...
- **Modular setup:**
roll your own

Runs on Linux, MacOS and Windows hosts using VirtualBox

Download: materialscloud.org/work/quantum-mobile

Future plans

- Open AiiDA lab for larger community (using federated authentication and Kubernetes for scaling)
- Migration to AiiDA 1.0
- Apps in preparation:
 - Cp2k workflows
 - Workflows to study gas adsorption
 - ...
- ...? - we are open for suggestions



Conclusions



- Workflows & Daemon help with automation
- AiiDA graph = map of the data jungle
- Your calculations are ready for Open Science



- Write simple apps in python
- Run where you like:
 - on your machine (your machine, your setup)
 - on Quantum Mobile (your machine, our setup)
 - on AiiDA lab (our machine, our setup)

Plans for the group work

- **Learn how to use Jupyter**
- **Learn how to use AiiDA lab**
 - Home page
 - App Store
 - App management
- **Learn about AiiDA lab internals (optional)**
 - AiiDA lab metapackage
 - AiiDA lab docker stack
 - AiiDA lab widgets base
 - AiiDA lab registry
- **Create your own AiiDA lab application**
 - Try out Cookiecutter to make your own app
 - Empower your app with AiiDA lab widgets
 - Run band structure workflow

Acknowledgements

Supported by



MARVEL NCCR
www.nccr-marvel.ch



MaX Centre
www.max-centre.eu



SNSF
<http://www.snf.ch>



EPFL
www.epfl.ch



CSCS
www.cscs.ch



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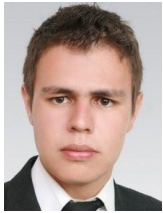


MarketPlace project
the-marketplace-project.eu



ERC
erc.europa.eu

Developers



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Contributors for the 23+ plugins: **Quantum ESPRESSO, Wannier90, CP2K, FLEUR, YAMBO, SIESTA, VASP, ...**

Contributors to aiida_core and former AiiDA team members — Valentin Bersier, Jocelyn Boullier, Jens Broeder, Andrea Cepellotti, Fernando Gargiulo, Dominik Gresch, Conrad Johnston, Rico Häuselmann, Eric Hontz, Christoph Koch, Espen Flage-Larsen, Antimo Marrazzo, Andrius Merkys, Nicolas Mounet, Tiziano Müller, Riccardo Sabatini, Ole Schütt, Phillippe Schwaller, Andreas Stamminger, Martin Uhrin, Spyros Zoupanos

The CSCS support teams

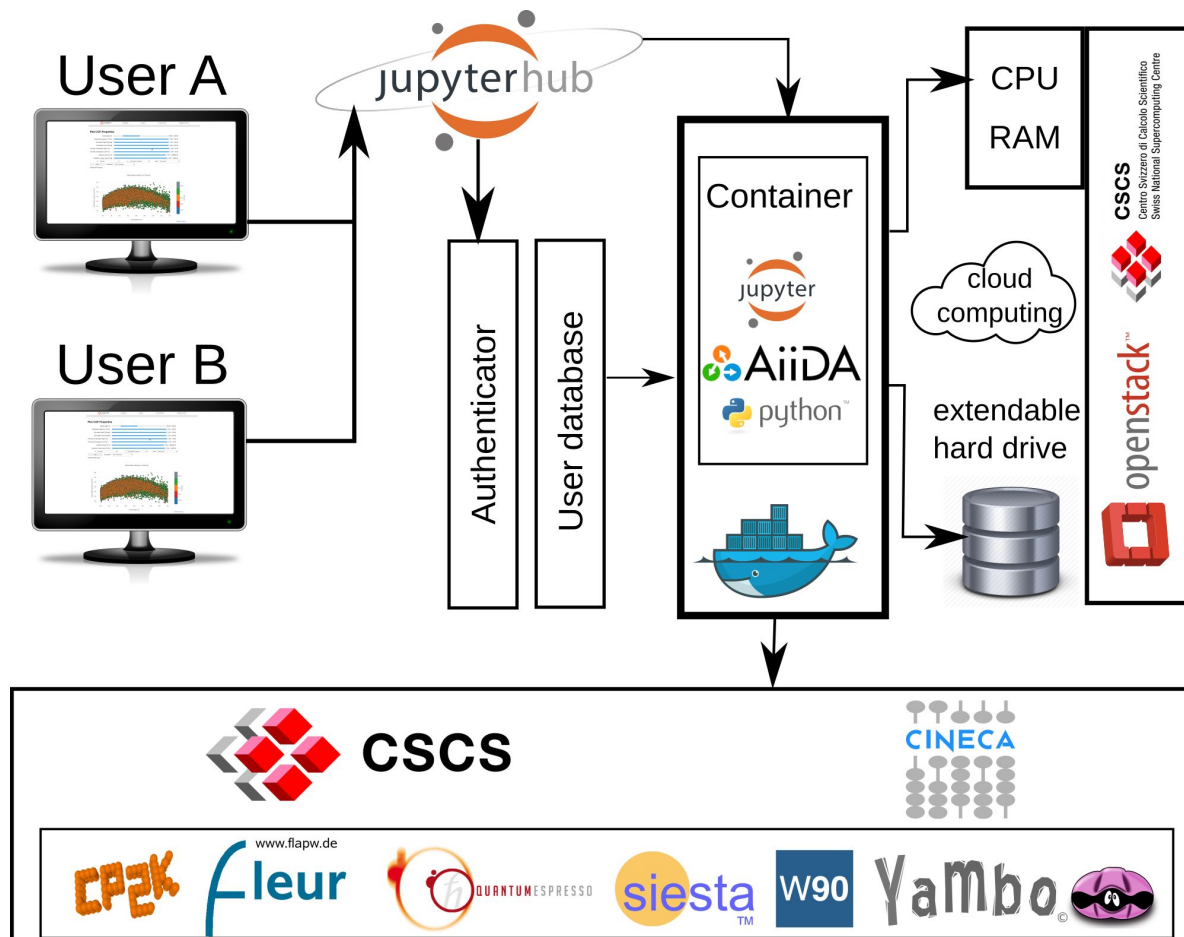
Interested in AiiDA lab?

Send us an email to:

aiidalab@materialscloud.org

and get your account today!

AiiDA lab Architecture



Technologies:

- JupyterHub (multi-user server for Jupyter notebooks)
- Jupyter notebooks (interactive python, + appmode)
- Docker (isolated environment for every user)
- Openstack (software to manage computing clouds)

Full list of plugins can be found on AiiDA plugin registry:
<https://aiidateam.github.io/aiida-registry>