AiiDAlab news

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AiiDAlab: Quick reminder

Three pillars of science

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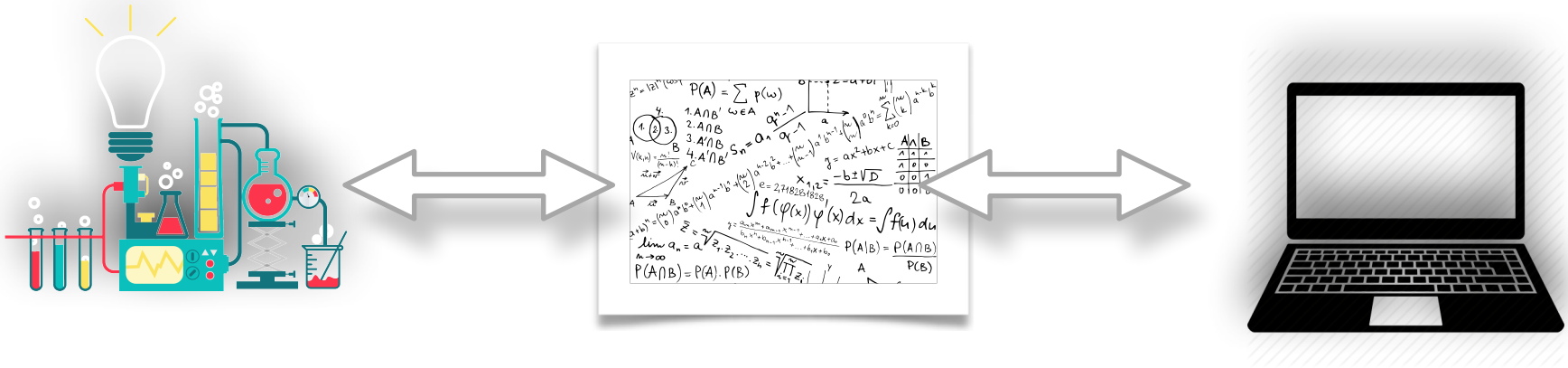
- Pillar I: Experiment. Mostly done by experimentalists.
- Pillar II: Theory. Mostly done by theoretical and computational scientists.
- Pillar III: Simulation: ~~Mostly done by computational scientists.~~

can be seen as a merging point between theory and experiment



AiiDA vs AiiDAlab

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AiiDA

Computational scientist

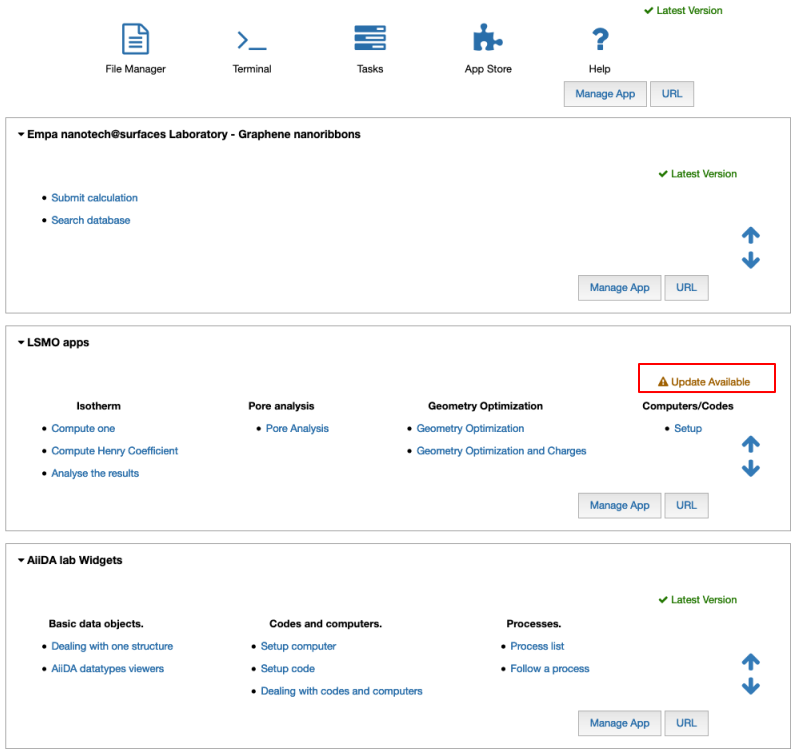
Computational/experimental scientist

AiiDAlab

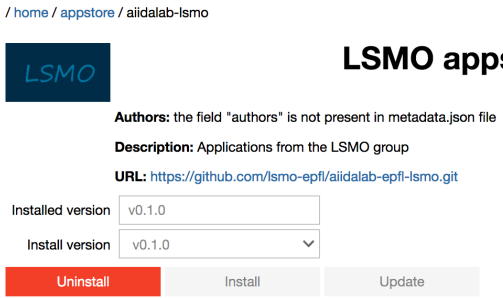
- Can run complex workflows
- Stores selected data
- Stores data provenance
- Has Python or command line interface

- Fully integrated with AiiDA
- User-friendly web interface (Jupyter notebooks & widgets)
- Easy application development (directly in Python)
- Collaborative environment.
- Handy visualization and editing tools
- App Store for sharing applications

AiiDAlab Home Page



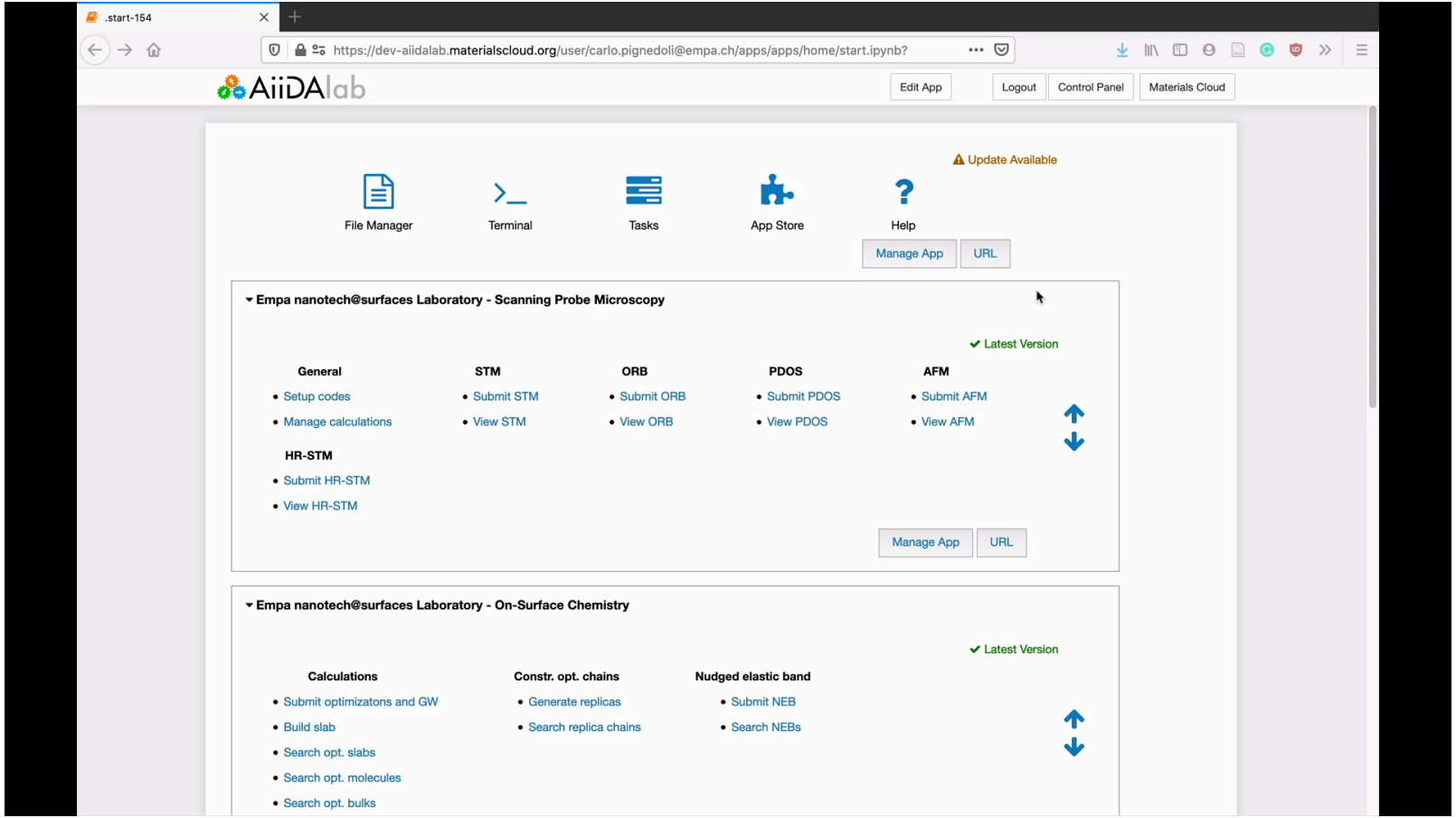
App Manager



Tight connection with Git for installation/deinstallation, update, version selection

GitHub **for sharing**

Usage example



AiiDAlab: status quo

Some statistics.

- Main AiiDAlab machine:
  - Total registered users **80**
  - Unique active users September: **14**
  - Hard drive space used: **693 GB/ 1200 GB**
- Open AiiDAlab machine (CESNET):
  - Total number of users who tried the service: **85**

News

- AiiDAlab paper is submitted (available on arXiv).
- The apps testing infrastructure is implemented.
- The maintenance of the service now takes much less time then before (before 1 day maintenance, now on the fly).
- Running AiiDAlab container locally is possible (Docker).
- New AiiDAlab machine in China (PARATERA organization, setup done by Jason Eu). AiiDAlab Marketplace is coming soon.

- **AiiDA lab is renamed to AiiDAlab.**

AiiDAlab paper

- Platform description:
  - Key components
  - Platform design
  - AiiDAlab distribution
- Use cases:
  - Computing electronic properties of GNRs.
  - On surface chemistry.
  - Scanning probe microscopy.

AiiDAlab – an ecosystem for developing, executing, and sharing scientific workflows

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Abstract

Cloud platforms allow users to execute tasks directly from their web browser and are a key enabling technology not only for commerce but also for computational science. Research software is often developed by scientists with limited experience in (and time for) user interface design, which can make research software difficult to install and use for novices. When combined with the increasing complexity of scientific workflows (involving many steps and software packages), setting up a computational research environment becomes a major entry barrier. AiiDAlab is a web platform that enables computational scientists to package scientific workflows and computational environments and share them with their collaborators and peers. By leveraging the AiiDA workflow manager and its plugin ecosys-

Testing infrastructure for the AiiDAlab apps

https://github.com/aiidalab/aiidalab-test-app-action

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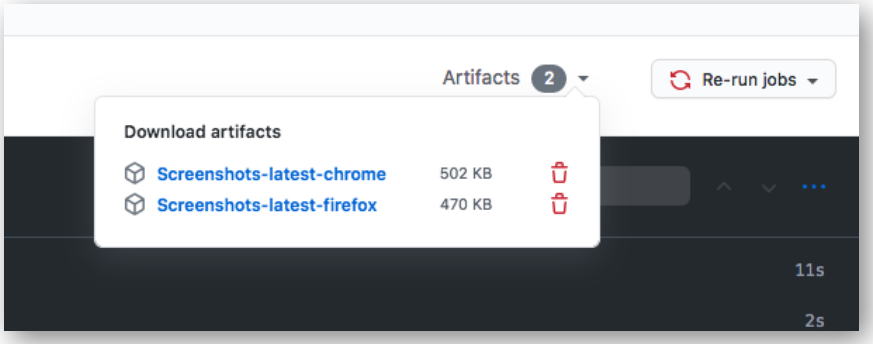
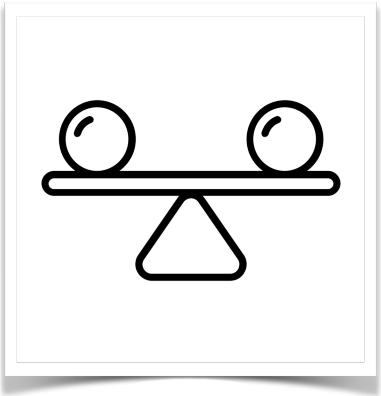
- **aiidalab-test-app-action**
  - Opens apps in different browsers (Chrome, Firefox).
  - “Clicks” on certain buttons.
  - Saves screenshots as GitHub artifacts.
  - Requires very minimal setup.





Stability

Kubernetes cluster problems

- Changing folder access permissions: .ssh, .postgres (cinder).
- K8s cluster node can’t have more than 6 volumes attached (cinder).
- Low performance when (nfs).
- PVC size limit is not respected (nfs).

Conclusion

- AiiDAlab is getting stable and much more maintainable: clear design, clear separation of concerns, auto-testing.
- New AiiDAlab machines: AiiDAlab in China (on), AiiDAlab Marketplace (soon).
- Shifting focus from the platform development to the apps development + providing documentation.
- Goal: running with 50 users connected at the same time.

Developers

The Materials Cloud And AiiDA teams


Carl Simon Adorf (EPFL)


Casper W. Andersen (EPFL)


Marnik Bercx (EPFL)


Marco Borelli (EPFL)


Valeria Granata (EPFL)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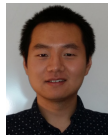
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Thomas Schulthess (ETHZ,CSCS)


Nicola Marzari (EPFL)

Contributors for the 40+ plugins: Quantum ESPRESSO, Wannier90, CP2K, FLEUR, YAMBO, SIESTA, VASP, CASTEP, CRYSTAL, …

Contributors to aiida-core and former AiiDA team members —
Oscar Arbelaez, Michael Atambo, Valentin Bersier, Marco Borelli, Jocelyn Boullier, Jens Bröder, Ivano E. Castelli, Andrea Cepellotti, Keija Cui, Vladimir Dikan, Marco Dorigo, Y.-W. Fang, Fernando Gargiulo, Marco Gibertini, Davide Grassano, Dominik Gresch, Conrad Johnston, Rico Häuselmann, Daniel Hollas, Eric Hontz, Jianxing Huang, Christoph Koch, Espen Flage-Larsen, Ian Lee, Daniel Marchand, Antimo Marrazzo, Andrius Merkys, Simon Pintarelli, Nicolas Mounet, Tiziano Müller, Gianluca Prandini, Philip Rüßmann, Riccardo Sabatini, Ole Schütt, Phillippe Schwaller, Andreas Stamminger, Atsushi Togo, Daniele Tomerini, Nicola Varini, Martin Uhrin, Jason Yu, Austin Zadoks, Bonan Zhu, Mario Zic, Spyros Zoupanos

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