

9:30-10:30

Introductory lecture

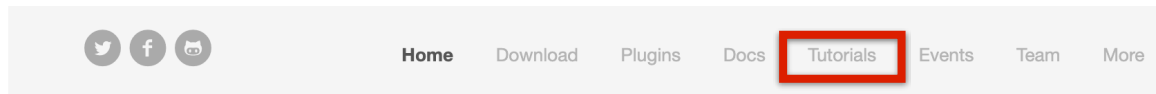
10:50-12:20Getting set up &
a "first taste" of AiiDA**12:20-14:00**

Lunch

14:00-15:50Extended AiiDA tutorial
Go at your own speed**16:10-17:10**Advanced tutorial continued
Available for Q&A

Tutorial Team

- Leopold Talirz (EPFL)
- Juson Yu (South China University of Technology)
- Yunpei Liu (Xiamen University)
- Jingfang Xiong (Xiamen University)




Automated Interactive Infrastructure and Database for Computational Science

AiiDA is a flexible and scalable informatics' infrastructure to manage, preserve, and disseminate the simulations, data, and workflows of modern-day computational science. Able to store the full provenance of each object, and based on a tailored database built for efficient data mining of heterogeneous results, AiiDA gives the user the ability to interact seamlessly with any number of remote HPC resources and codes, thanks to its flexible plugin interface and workflow engine for the automation of complex sequences of simulations.

Journal ref: G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, and B. Kozinsky, AiiDA: automated interactive infrastructure and database for computational science, *Comp. Mat. Sci.* 111, 218-230 (2016)

Open access link: [arXiv:1504.0116](https://arxiv.org/abs/1504.0116)

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TUTORIAL MATERIALS

2019, Xiamen University, China (aiida-core 1.0.0b6)

2019, EPFL, Switzerland (aiida-core 1.0.0b3)

2019, University of Amsterdam, Netherlands (aiida-core 0.12.2)

2018, Cineca, Italy (aiida-core 1.0.0a1)

2018, EPFL, Switzerland (aiida-core 0.11.4)

2017, EPFL, Switzerland (aiida-core 0.9.0)

2017, ICTP, Italy (aiida-core 0.7.1)

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AiiDA Tutorials

The official place to find materials from AiiDA tutorial events, interactive demos and videos.

Tutorial materials

- 2019, Xiamen University, China (aiida-core 1.0.0b6)
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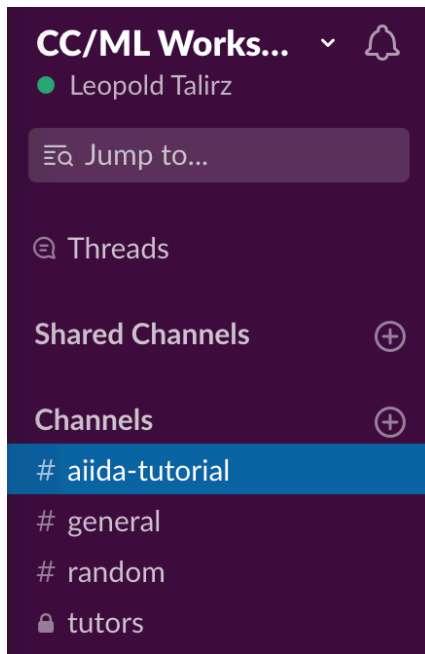
Get a GitHub account!
report issues, fix typos, ...
we love pull requests :-)

Tutorial materials

- [2019, Xiamen University, China \(aiida-core 1.0.0b6\)](#)
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Important information

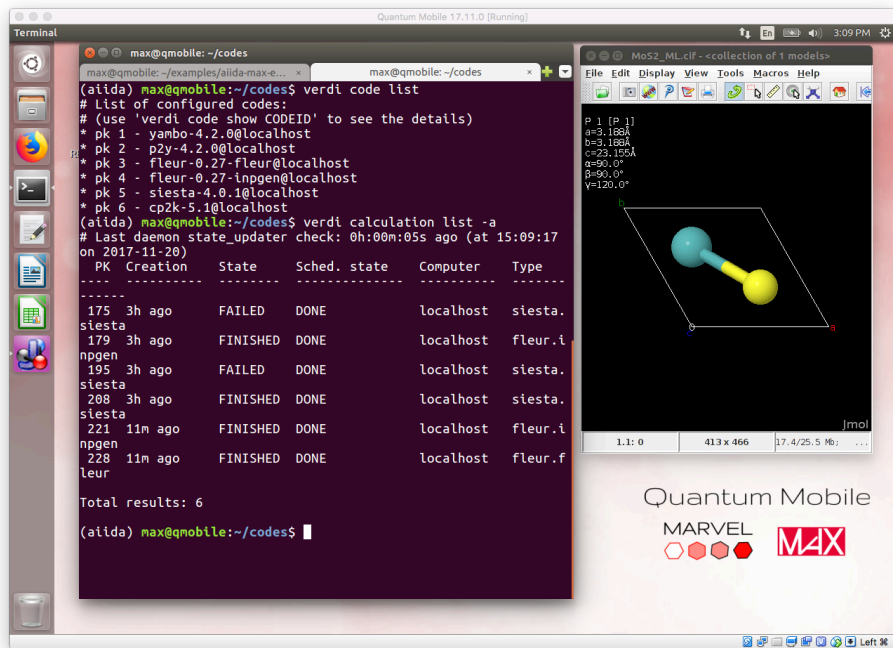


- If possible, **create a WiFi hotspot using your phone** - it seems Huawei cloud blocks when too many use the local WiFi
- Feel free to ask questions on slack
invite link: dwz.cn/WPlahDr5
(capital i, not lowercase L)
- **Password for "max" user of your tutorial virtual machine**
XMNAiIDA2019

Questions?



Quantum Mobile Virtual Machine



- Ubuntu 18.04 LTS
- AiiDA & AiiDA Lab
- Open-source codes:
Quantum ESPRESSO, Siesta,
fleur, yambo, cp2k, Wannier90
+ AiiDA plugins
- Great for tutorials & lectures
(EPFL, ETHZ, ICTP, MolSim and
online classes: compmatphys.org)
- Modular setup using ansible

Runs on any Linux, MacOS and Windows hosts using VirtualBox

Download: materialscloud.org/work/quantum-mobile