



# AiiDA lab

Aliksandr Yakutovich



# AiiDA vs AiiDA lab



Computational scientist



Computational/experimental  
scientist



- 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 visualisation and editing tools
- App Store for sharing applications

- [done] Preparation work:
  - Integration with EGI Check-in.
  - Support for AiiDA  $\geq 1.1$ .
- [done] Q2:
  - Increase capacity at CESNET to support at least 50 users.
  - Move to EGI Check-in production instance.
  - Deployment of an application to run Quantum ESPRESSO relaxation workflows.
- [in progress] Q3:
  - On-boarding of users (~50 expected) [issues]
  - Installation in the instance of updated apps, software stack and data as needed for a tutorial [in progress]

- When ~10 users are connected at the same time, k8s nodes fail. Enol is investigating this.
- After restarting a node, the permissions to the folders are overwritten. Especially problematic for ~/.ssh and ~/.postgresql folders

- Install apps' dependencies. Currently all the apps' dependencies are installed with the aiidalab python package
- Stabilizing/testing the apps. The testing infrastructure is developed.
- AiiDA lab documentation.
- Sharing data among users.
- Provide straightforward apps to connect to HPC resources.