EGI-ACE Open Call no.1

Checkpoint meeting with Shepherds

Open AiiDAlab platform for cloud computing in Materials Science

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Dissemination level:

Disclosing Party:

Recipient Party:

Background about the scientific use case

The goal of AiiDAlab is to make simulations accessible. AiiDAlab provides a user-friendly interface to AiiDA that manages complex workflows to run simulations. It also leverages a great variety of python-based tools that allow prepare simulation inputs in a straightforward manner.

- Currently focused on Materials Science but can be extended to other fields.

- Main users of the platform:
    - EPFL: THEOS (prof. Nicola Marzari, Lausanne) and LSMO (prof. Berend Smit, Sion) laboratories.
    - Empa: nanotech@surfaces (prof. Roman Fasel, Dübendorf).
    - Coming soon: Paul Scherrer Institute (Switzerlnad)

- Key partners:
    - Swiss National Supercomputing Centre (Lugano).
    - MARVEL National Centre for Competency in Research (Switzerland).
    - MaX European Centre of Excellence.
    - Swiss National Science Foundation.

Ambition, Impact, Challenge(s)

The goal of AiiDAlab is to make simulations accessible. AiiDAlab provides a user friendly interface to AiiDA that manages complex workflows to run simulations. It also leverages a great variety of python-based tools that allow prepare simulation inputs in a straightforward manner.

Our ambition is to make AiiDAlab a widely used platform that helps scientists in daily research. For this we would like to make the entry barrier to AiiDAlab as low as possible. We are trying to achieve that by:

- Having a demonstration server that can be used by the potential users for testing.
- Run schools and tutorials on the publicly available AiiDAlab.

Having a **scalable instance** that is easily accessible and can be used by many people in the same time is an important requirement to achieve our goals.

Integration Support

We hope that EGI-ACE will be able to help us to procure the resources needed to rapidly scale up this demonstration service such that we can comfortably advertise it to the general scientific community.

We anticipate that for this we will need to support at least 100 concurrently active user sessions at peak times and on the order of 500 user accounts in total (a ten-fold increase).

Need:
- Stable Kubernetes deployment – operated and maintained by the providers as much as possible
- Enough capacity for deploying production + testing instances of the service
- Auto-scalable setup to support peaks (e.g. training events) and avoid pre-reserving resources that will sit idle most of the time

Capacity Requirements

Kubernetes cluster with (peak):
- 100 CPU cores
- 400 GB RAM
- 8 TB storage space.

Per user:
- 1 CPU core
- 4 GB of RAM
- 20 GB storage space

Timeline

Current Status:
- aiidalab-demo is production-ready and deployed at CESNET
- New features are introduced continually into the service (e.g. improved applications dependency management)
- Aiidalab-demo is already in EOSC marketplace: https://marketplace.eosc-portal.eu/services/aiida-lab

Next steps:
- Scalable k8s setup with EC3 (Q4 2021)
- integration with EGI notebooks (Q1 2022)

Dissemination activities:
- AiiDA tutorial was fully run on AiiDAlab: https://aiida-tutorials.readthedocs.io/en/tutorial-2021-intro/
- Computational methods in chemistry course, EPFL: https://edu.epfl.ch/coursebook/en/computational-method-in-chemistry-and-chemical-engineering-data-in-chemistry-and-electronic-lab-notebooks-CHE-609-4

Thank you!

Contact: **egi-ace-po@mailman.egi.eu**
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