

CR: Open AiiDALab platform for cloud computing in Materials Science (EAP)

Short description	The AiiDALab brings the AiiDA workflow manager for computational science (www.aiida.net) to the cloud. The AiiDALab web platform gives novice users access to their personal pre-configured AiiDA environment in the cloud. The AiiDALab uses docker for user containers, and kubernetes for orchestration. Users get persistent home volumes for active use (no long-term storage component).
Type of community	Others (EAP)
Community contact	Leopold Talirz <leopold.talirz@epfl.ch>
Interviewer	Enol Fernandez del Castillo
Date of interview	2020. 4. 27
Meetings	
Supporters	

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User stories



Instruction

Requirements are based on a user story, which is an informal, natural language description of one or more features of a software system. User stories are often written from the perspective of an end user or user of a system. Depending on the community, user stories may be written by various stakeholders including clients, users, managers or development team members. They facilitate sensemaking and communication, that is, they help software teams organize their understanding of the system and its context. Please do not confuse user story with system requirements. A user story is an informal description of a feature; a requirement is a formal description of need (See section later).

User stories may follow one of several formats or templates. The most common would be:

"As a <role>, I want <capability> so that <receive benefit>"

"In order to <receive benefit> as a <role>, I want <goal/desire>"

"As <persona>, I want <what?> so that <why?>" where a persona is a fictional stakeholder (e.g. user). A persona may include a name, picture; characteristics, behaviours, attitudes, and a goal which the product should help them achieve.

Example:

"As provider of the Climate gateway I want to empower researchers from academia to interact with datasets stored in the Climate Catalogue, and bring their own applications to analyse this data on remote cloud servers offered via EGI."

No.	User stories
US1	As a computational scientist I want to login into the AiiDALab using my institutional credentials.
US2	As a computational scientist, I need to have a personal space to store data that persist between logins.
US3	As a materials scientist I would like to use the AiiDALab to run and manage materials science workflows on remote compute resources.
US4	As a computational scientist I would like to use the AiiDALab to participate in AiiDA tutorials so that I do not need to set up the software on my local machine.

Use cases



Instruction

A use case is a list of actions or event steps typically defining the interactions between a role (known in the Unified Modeling Language as an actor) and a system to achieve a goal.

Include in this section any diagrams that could facilitate the understanding of the use cases and their relationships.

Step	Description of action	Dependency on 3rd party services (EOSC-hub or other)
UC1	Access via institutional credentials to the service	EOSC-hub AAI
UC2	Provide an online version of AiiDA Lab completely accessible via browser that does not require installation of software	
UC3	Access to a persistent storage pool for users personal space	EGI Online Storage
UC4	Access to compute resources to run users workload	EGI Cloud Compute
UC5	Provide a kubernetes deployment to manage access to compute and storage resources for the application	EGI Cloud Container Compute
UC6	Provide scalable kubernetes setup that can adapt to workload during trainings	EC3

Requirements


Technical Requirements



Instruction

- Requirement number: Use numbers RQ1, RQ2, RQ3, ...
- Requirement title: Use a short but descriptive title. Use the same title in the Jira ticket 'Summary' field
- Link to requirement JIRA ticket: Open a ticket in <this JIRA queue <https://jira.eosc-hub.eu/projects/EOSCWP10/issues/EOSCWP10-4?filter=allopenissues>> (click on 'CREATE' button in the middle-top of JIRA)
- Source use case: Refer back to the use cases above (UC1, 2, ...)

Requirement number	Requirement title	Link to Requirement JIRA ticket	Source Use Case
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Example	EOSC-hub to provide an FTS data transfer service	 EOS CWP 10- 21 - Jira 	UC1
RQ1	EOSC-hub to provide a kubernetes managed pool of resources to deploy AiiDA lab		UC5, UC6
RQ2	EOSC-hub to provide a single sign-on services that supports institutional credentials		UC1
RQ3	EOSC-hub to provide a scalable kubernetes cluster to accommodate varying load during training events		UC6
RQ4	EOSC-hub to provide enough resources to host planned training events		UC2, UC3, UC4

Capacity Requirements

EOSC-hub services	Amount of requested resources	Time period