Contribution ID: **1**   Type: **not specified**

AiiDA Lab –an Ecosystem for Developing, Executing and Sharing Scientific Workflows

Thursday, 22 October 2020 10:45 (30 minutes)

Computational simulations constitute an integral part of modern science. Running scientific software, however, requires expert knowledge not only in the modelled scientific phenomena but often also in accessing and operating compute resources, programming, installing and compiling software, and other topics related to computation. In the presentation I will introduce AiiDA lab, an open source platform that provides the means to develop, execute and share computational science workflows as an intuitive web service available to anyone who knows how to use a web browser. AiiDA lab is built on top of AiiDA, an infrastructure that provides the automatic workflow engine and provenance tracking, and Jupyter, which powers the graphical user interfaces.

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