

AiiDALab –an Ecosystem for Developing, Executing, and Sharing Scientific Workflows

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Cloud platforms allow users to execute tasks directly from their web browser and are a key enabling technology not only for commerce but also for computational science. Research software is often developed by scientists with limited experience in (and time for) user interface design, which can make research software difficult to install and use for novices. When combined with the increasing complexity of scientific workflows (involving many steps and software packages), setting up a computational research environment becomes a major entry barrier.

AiiDALab is a web platform that enables computational scientists to package scientific workflows and computational environments and share them with their collaborators and peers. By leveraging the AiiDA workflow manager and its plugin ecosystem, developers get access to a growing range of simulation codes through a python API, coupled with automatic provenance tracking of simulations for full reproducibility.

Computational workflows can be bundled together with user-friendly graphical interfaces and made available through the AiiDALab app store. Being fully compatible with open-science principles, AiiDALab provides a complete infrastructure for automated workflows and provenance tracking, where incorporating new capabilities becomes intuitive, requiring only Python knowledge.

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