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Complex workflows in modern computational science using AiiDA and HELIPORT

AiiDA is an open-source Python infrastructure for devising complex workflows associated with modern computational science and streamlining the four core pillars of the ADES model: Automation, Data, Environment, and Sharing. In this contribution, we showcase features of AiiDA like workflow-forging, high-throughput capability and data provenance as implemented in the AiiDA-FLEUR plugin. Finally, we address the possibility of managing AiiDA-projects through HELIPORT.

Speed Talks

Normal

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