

Programme and location

The programme includes a tutorial on the AiiDA code, and two scientific talks on their research using AiiDA for high-throughput computations:

Giovanni Pizzi (EPFL, Lausanne, Switzerland)

Title: Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds

Leonid Kahle (EPFL, Lausanne, Switzerland)

Title: Fast screening of solid-state lithium-ion conductors

The tutorial will take place at CINECA, near Bologna in Italy. It will start on Wednesday May 30, 2018 (at 9:00 AM) and will finish on Friday June 1, 2018 (at 12:30 PM).

Programme Day 1 (Wednesday)

Morning

- 09:00 – 09:30 Registration
- 09:30 – 09:50 Introduction by the organizers
- 09:50 – 10:30 Introductory talk on high-throughput computations and AiiDA (Spyros Zoupanos – 30 minutes + 10 minutes)
- 10:30 – 11:00 Coffee break
- 11:00 – 12:30 Hands-on tutorial on provenance-aware scientific computing. Topics: Introduction to provenance & database-backed provenance tracking, exploring the provenance graph.
- Lunch

Afternoon

- 14:00 – 16:00 Hands-on tutorial on simulation submission using AiiDA. Topics: calculations submission preparation, use of Quantum ESPRESSO plugin, submission monitoring and debugging.
- 16:00 – 16:30 Coffee break
- 16:30 – 18:30 Hands-on tutorial on simulation result and provenance graph analysis. Topics: Understanding QueryBuilder, writing graph queries, using QueryBuilder to analyse your research
- 18:30 – 19:00 Setup of posters

Programme Day 2 (Thursday)

Morning

- 9:00 – 10:00 Scientific talk "Discovering two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds" by Giovanni Pizzi (EPFL, Lausanne, Switzerland) (45 minutes + 15 minutes for questions)
- 10:00 – 10:30 How to achieve FAIR sharing and write DMPs with AiiDA and the Materials Cloud (20 minutes + 10 minutes for question)
- 10:30 – 11:00 Coffee break
- 11:00 – 12:30 Hands-on tutorial on simulation result and provenance graph analysis (continued)
- Lunch

Afternoon

- 14:00 – 16:00 Hands-on tutorial on automated workflows. Topics: Orchestrating simulations using workflows; enhanced provenance; how

to use and write workflows.

- 16:00 – 16:30 Coffee break
- 16:30 – 17:30 Hands-on session on automated workflows. Topics: workflows in AiiDA – WorkChains and WorkFunctions
- 17:30 – 19:00 Poster session by the participants with social dinner (standing buffet).

Programme Day 3 (Friday)

Morning

- 9:00 – 10:00 Scientific talk "Fast screening of solid-state lithium-ion conductors" by Leonid Kahle (EPFL, Lausanne, Switzerland) (45 minutes + 15 minutes for questions)
- 10:00 – 12:00 Hands-on session on automated workflows. Topics: workflows in AiiDA – WorkChains and WorkFunctions (continued)
- 12:00 – 12:30 Coffee with Final discussions & closing remarks by the organizers
- Lunch (optional)