The Abdus Salam International Centre for Theoretical Physics

College on Multiscale Computational Modeling of Materials for Energy Applications
4 - 15 July 2016

Co-sponsors: INRS Canada, ESF and Psi-k

Managing Computational Materials Science: The ADES Model and the AiiDA Infrasture

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Abstract:

Thanks to the advances in simulation codes and the increase in computational power, "Materials by design" has become a powerful approach in Materials Science. This approach often requires to run large numbers of simulations and to build databases of computed properties. A key challenge is the need to automatically prepare, execute and monitor workflows of calculations, and then retrieve and store the results in a format easy to browse and query. Such materials' informatics platform should offer a fast learning curve, and encourage sharing of codes, results and workflows. After having enshrined these needs in the four "ADES" pillars of Automation, Data, Environment, and Sharing, we have implemented them in the open-source AiiDA platform [1] (http://www.aiida.net) whose design, based on directed acyclic graphs, aims at guaranteeing provenance, preservation, and searchability of heterogeneous data. This talk will introduce the basic concepts used in AiiDA (graph database for the representation of the provenance, queries, workflows, …) that we will then learn to use during the hands-on session.

[1] G. Pizzi et al., Comp. Mat. Sci. 111, 218-230 (2016)