

Scientific workflows with FireWorks

Thursday, August 31, 2017 1:00 PM (5 hours)

Scientific workflow is an important technique used in many simulation and data analysis applications. In particular, workflows automate high-throughput / high-complexity computing applications, enable code and data reuse and provenance, provide methods for validation and error tracking, and exploit application concurrency using distributed computing resources. The goal of this tutorial is to learn composing and running workflow applications using the FireWorks workflow environment (<https://hackingmaterials.lbl.gov/fireworks>). In the first part, after an introduction to the concept of workflows, to state-of-the-art workflow systems and to FireWorks, the participants will learn to construct workflows using a library of existing Firetasks. The composed workflows will be verified, visualized and then executed and monitored. The included exercises will include managing data and control flow dynamically using FWAction. The second part will focus on writing custom Firetasks to match more specific application requirements. Basic knowledge of using the bash shell is required. For the second part, basic knowledge of Python is required.

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Session Classification: Tutorials