

Interfacing AiiDA to FirecREST: A RESTful Approach to HPC Workflows

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In today's supercomputing landscape, securing both computational resources and results has become increasingly important. Usually, HPC systems are interfaced with users via SSH. However, due to security vulnerabilities and the expensive costs of login servers, many supercomputing centers are now exploring modern alternatives.

One promising alternative is to adopt REST API-based solutions to manage HPC resources. While such APIs provide enhanced security and lower operational costs, they also introduce challenges due to increased latency of REST compared to SSH. This performance limitation might present a challenge for developers of large-scale, high-performance workflow managers, such as AiiDA, to redesign their systems in ways that handle server communication delays efficiently.

This presentation will explore how AiiDA, as a high-performance workflow manager, has been adapted to interface with FirecREST—a REST API-based interface for managing HPC resources. I will discuss some of the technical challenges we faced and how we addressed them to maintain performance.

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