AI-Science for Performance Optimization and Diagnosis of Science Instrument Federations

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Introduction: Next generation of science workflows are expected to be executed over complex federations composed of supercomputers, science instruments, storage systems and networks, with new additions of the edge and cloud systems and services. The sheer complexity of these multi-domain federations makes it hard to manage them and optimize their performance, as small impedance mismatches (that can dynamically develop between systems) could drastically degrade the entire federation performance. Recent proliferation of Software Defined Everything (SDX) technologies combined with containerization frameworks provide custom instruments that can monitor and collect critical measurements at various levels to support diagnoses and performance optimization; but their data too enormous for human operators and analysts to process and generate decisions. Machine Learning (ML) methods that extract critical parameters, relationships and trends from the data offer general solutions. Artificial Intelligence (AI) and ML methods must be custom-developed for these problems based on solid, rigorous foundations, since black-box approaches are often ineffective and unsound.

AI-Science for measurements driven science federations: We propose to develop comprehensive AI-Science for the performance of science federations to (i) monitor and control storage, networks, experiments, and computing systems across multiple domains via softwarization layers, at speeds and scales orders of magnitude superior to current practice, (ii) optimally realize and orchestrate complex workflows with high performance by using dynamic state and performance estimation methods, and (iii) aggregate measurements across sites and time to develop infrastructure-level profiles, optimizations and diagnoses using AI-Science based on foundational principles from ML, game theory, and information fusion areas. This approach provides measurements driven, performance optimized science federations with following capabilities:

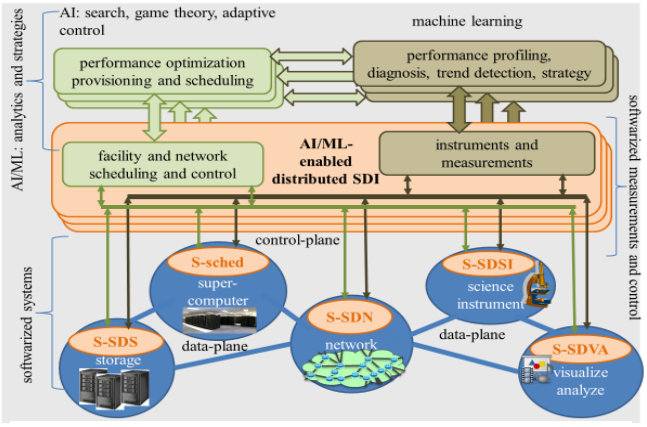

Figure 1. AI-Science driven science federation.

- *Self assessment Using Performance Profiling:* Automated, adaptive collection of data from many devices and at multiple levels, and AI-driven integration into dynamic performance profiles; and
- *Continuous Performance Optimization*: Sustained performance optimization using trend detection and strategy adaptation based on measurement streams using performance analytics and game theory.

RoadMap: We propose a long-term strategy to continuously build upon a spectrum of technologies and foundational principle from SDX and AI/ML area in the following topics shown in Figure 1:

- **Integrated instruments and measurements**: We propose a comprehensive SDX and container-based measurement framework by leveraging domain tools for devices, systems, facilities, workflows, and infrastructure. We propose to develop custom AI/ML methods for optimal monitoring, and ML methods for short- and long-term performance profiling.
- **Performance optimization for science users and facility providers**: By building performance profiles and identifying optimal configurations in multi-system joint parameter space, we propose workflow composition and optimal mapping methods using resource objects, implement them using distributed SDX control mechanisms, and monitor them under the measurement infrastructure.
- **Performance analytics and strategies**: We propose practical AI-based analytics based on foundational principles to integrate measurements across facilities and time for (a) performance monitoring and diagnosis using incipient fault detection, information fusion methods, (b) trend detection at sites using ML (e.g. SVM, random forest, deep learning, and others) methods, and (c) decision making and game theoretic strategies for performance optimization at infrastructure level.