

Event-Driven Foundations of Autonomy: Laboratories and Digital Twins

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Abstract

Autonomous laboratories and executable digital twin environments demand more than automation—they require connected, intelligent cyberinfrastructure built on bidirectional data flow, semantic integration, and knowledge-based reasoning. In such complex environments, event-driven architecture serves as the foundational design principle. Event-driven approaches enable next-generation platforms with orchestration of complex, distributed workflows across instruments, computational models, and decision-making agents.

In this presentation, we detail our mission-driven development of an event-based approach within the AIMD-L (Artificial Intelligence for Materials Design Laboratory) and IMQCAM (Institute for Model-based Qualification and Certification of Additive Manufacturing) projects. This includes novel uses of our OpenMSIStream streaming framework, workflow orchestration through data portals, and emerging strategies for globally unique, persistent identifiers (PIDs) for physical samples. These tools enable real-time coordination of heterogeneous scientific components, paving the way for agile, model-centric experimentation.

Beyond infrastructure, a central challenge in achieving autonomy is representing knowledge in a form that supports both scientific discovery and intelligent decision-making. We address this by adopting the graphical expression of materials data (GEMD) as a canonical, machine-readable structure to represent material histories, synthesis and processing steps, and characterization events. GEMD captures causal relationships across workflows, enabling provenance-aware, AI-ready experimentation.

As we move forward, we are exploring the integration of GEMD with semantic technologies and traditional RDF-based knowledge graphs, enabling hybrid reasoning systems that support adaptive decision-making, explainability, and closed-loop optimization. Together, these developments form a flexible, event-driven foundation for autonomous science platforms and certifiable digital twins in materials science.