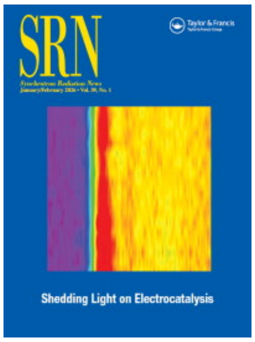


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# Agentic AI for User Facilities: Workshop Report

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# Agentic AI for User Facilities: Workshop Report

## Executive summary

This workshop addressed a gap: the most recent DOE reports on AI for science [1–3] predate recent advances in agentic AI—LLM-based systems that can plan, orchestrate, and execute multi-step workflows. With 100 participants from eight US DOE facilities and two allied facilities across accelerators, beamlines, nanoscience, genomics/biology, and computing infrastructure, this report identifies paths to deploy agentic AI at DOE user facilities while preserving safety, accountability, and rigor. Discussions also reflected DOE's Genesis mission emphasis on end-to-end workflow acceleration through integrated data, computing, and AI capabilities.

### *Key findings*

(1) The participants identified numerous areas where agentic AI could offer significant value to DOE user facility operations (2) The "co-pilot" model, where agents recommend actions but require human approval for consequential steps, emerged as the consensus design pattern across all domains. Default read-only access with human-gated write operations addresses safety concerns while delivering immediate value. (3) Treating agents as a subset of the capabilities of authenticated facility users with delegated capabilities within existing access-control frameworks, rather than privileged automation, provides a governance model for safe deployment. (4) Evidence-based deployment: as emphasized across multiple working groups, participants called for reproducible, domain-scientist-evaluated demonstrations (often progressing from simulation to live instruments) and step-change (i.e., "10X") improvements to justify adoption costs.

### *Critical gaps*

Machine-accessible knowledge is the highest-value gap. Both structured data standards and tacit subject matter expert (SME) knowledge (e.g., protocols, procedures, and experimental context) must be captured in machine-readable formats. Observability and traceability are essential: comprehensive logging of what agents read from data, write to configuration, execute, and resulting artifacts enables trust, debugging, and evaluation. Digital twins, ranging from fast "primitive simulations" to robust high-fidelity versions provide critical safe staging environments to validate agent actions before production deployment. How to address skill atrophy, when operators lose manual expertise and automation fails, represents a structural risk that requires proactive mitigation and research. Authentication and authorization for autonomous agents remain active areas, with promising approaches emerging; interoperable, auditable delegation for long-running, cross-facility workflows remains a key challenge.

### *Strategic direction*

DOE should prioritize areas where it has unique competitive advantage, including cross-facility coordination infrastructure (American Science Cloud (AmSC), federated agent registries, and shared tool registries all validated by cross-site conformance tests), safety-critical agentic architectures transferable to other high-consequence domains, and scale integration across DOE datasets, HPC, and experimental facilities. Frontier model development and general-purpose agentic frameworks should be left to industry; DOE's role is scalable, integratable, governance, and domain adaptation of models and agentic frameworks. Leadership must also mandate policies preserving human expertise alongside automation; skill atrophy is the most critical structural risk identified.

## Workshop overview

The workshop was convened January 21–22, 2026, at Lawrence Berkeley National Laboratory. The first morning featured plenary talks. Participants then split into topic-based breakouts: semantic understanding and knowledge; models and reasoning; agent architectures and design patterns; and tools, interfaces, and integration. The second morning organized participants into domain-based breakouts: accelerators and control systems; beamlines and experimental stations; computing and AI infrastructure; and nanoscience, biology, and chemistry. Each session concluded with cross-group report-outs, and the final afternoon was devoted to collaborative synthesis of this document.

## Domain priorities, opportunities, and readiness

### *Accelerators*

Agentic AI targets key pain points in accelerator operations: fault diagnosis, root cause analysis, and routine tuning that consume expert attention. This domain is characterized by a small number of highly unique, capital-intensive machines with long lifetimes and high consequences of error, making reliability, provenance, and access control first-order requirements rather than optimizations. Current readiness is low—operators struggle to locate relevant control variables, logs, and procedures across fragmented data systems. A risk-averse operating culture

*Plenary session.*

*Breakout sessions.*

requires proven reliability before granting control authority. The recommended path forward is a copilot model, implemented as a facility-managed service with controlled tool access: agents aggregate context across tools and time, detect anomalies via historical comparison, assist during faults, and provide read-only analytics. Where agents propose operational changes, execution remains explicitly human-gated. This environment particularly benefits from shared cross-facility frameworks (authentication, auditability, conformance tests) that reduce duplication while respecting machine-specific constraints. Success metrics should center on operational impact: measurable downtime reduction, faster fault recovery, and demonstrable separation between AI systems and hardware protection layers.

***Beamlines and experimental stations***

Increasing detector speeds, data volumes, and instrument complexity are stretching human-centric workflows for experiment planning, execution, and analysis. Promising agent workflows include end-to-end experiment coordination: querying materials databases, combining simulations with AI for parameter selection, autonomous alignment, generating control-system plans, and adaptive real-time analysis. Agents can also assist proposal development and feasibility assessment via digital twin integration. A key architectural principle is that agents should operate with user-delegated capabilities, equivalent to those of authenticated facility users, and remain governed by existing identity, authentication, and role-based access control frameworks rather than being deployed as privileged automation. This includes beamtime-bounded scope, risk-appropriate authority levels, and full provenance for auditability. Currently, readiness to adopt AI is overall moderate but disparate across and within the labs; widespread adoption requires investment to provide interfaces, standardize metadata, automate rich and consistent electronic logbooks, and AI-aware design principles.

***Nanoscience, biology and chemistry***

These domains are characterized by smaller individual datasets but enormous aggregate complexity from the diversity of materials and heterogeneity of measurement techniques. The defining challenge: users bring externally prepared samples with unknown histories, creating fundamental gaps in the experimental context. Systematic metadata capture emerged as the critical priority—agents observing human processes or logging robotic workflows can assist transforming context-poor data into ML-ready datasets with complete sample genealogy. Template-based planning is the preferred approach: conversational agents that guide users through validated recipes while tracking deviations. Multi-agent architectures suit this domain's heterogeneity, with specialized agents for different instruments integrating results across modalities. A pragmatic near-term enabler is using "primitive simulations" (or partial digital twins) to validate agent plans and quality controls before interacting with real instruments. Key infrastructure gaps include vendor-limited APIs, knowledge graphs encoding procedures, and data policy frameworks for user consent.

***Computing and AI infrastructure***

DOE facilities operate a compute ecosystem: facility-edge computing, leadership HPC centers, hybrid cloud, and ESnet coordination. Current readiness varies across sites—monitoring, logging, containers, and facilities/scheduling APIs exist but remain inconsistent across sites. A major bottleneck for integrating computing facilities with beamlines and accelerators remains tacit knowledge held by subject matter experts (SMEs) e.g., naming conventions for sensors, magnets, etc. The critical barrier is authentication and authorization for autonomous agents, particularly for long-running, cross-facility workflows requiring persistent identity, scoped authority, and auditable access. The recommended approach is a planning-first model: agents propose and validate execution plans for human approval before acting on shared infrastructure. Lastly, standardized APIs, consistent containerization, agent registries, and multi-facility conformance tests demonstrating reproducible

*Collaborative report writing session.*

workflow execution across heterogeneous sites will enable cross-facility sharing and deployment of agentic capabilities.

## Cross-cutting priorities and enablers

### *Models and reasoning*

LLMs are effective for initial literature search, experimental configuration, and implementing parameter space exploration. However, validation and verification remain fundamental challenges. Citation hallucination poses risks for scientific applications, where agents may fabricate references with high confidence. Mitigating these risks requires linking/publishing raw data alongside processed results and implementing verification workflows that distinguish retrieved from generated content. Until models can reliably express uncertainty, human oversight of factual claims remains essential.

### *Agentic frameworks*

Strong consensus formed around a "co-pilot" design pattern, where agents recommend actions but humans approve high-impact steps. Recommended safety practices include:

- **Strict separation of planning and execution** phases
- **Read-only access by default** with human-gated write operations
- Layered verification combining LLM red-teaming with experimental validation
- Containerization to enforce effective resource protection (e.g., cgroups, namespaces)
- Role-based access control to prevent privilege escalation

Production platforms like Osprey [4] demonstrate viability, with Model Context Protocol (MCP) servers enabling integration across control systems and HPC operations through controlled tool interfaces and auditability. Across discussions, participants emphasized that shared, facility-managed agent services and reusable tool ecosystems can reduce duplication, improve maintainability, and accelerate safe deployment across sites. Related scalable agentic frameworks (e.g., Academy [5]) and self-hosted inference services (e.g., vLLM) were discussed as practical components for facility deployments.

### *Human-agent collaboration*

Human-agent collaboration is already operational but narrowly scoped. Production systems at Diamond Light Source (such as CHiMP on VMXi, automating crystal scanning at ~98% accuracy; Bayesian bimorph mirror piezo optimization reducing day-long procedures to ~10 minutes) and at Argonne (APEXA orchestrating HEDM analysis via peer-reviewed tools through MCP) illustrate that trust increases when agents route work through familiar software with end-to-end traceability. Adoption still requires improvements; step-function (e.g., 10X) gains, not incremental gains, are needed to overcome organizational inertia. Key risks include skill atrophy (automation complacency), the challenge of ensuring safe operation during off-hours by minimally trained visiting users, and adoption fragility following a single high-profile failure. Security and privacy constraints (e.g., FedRAMP/vendor limits; camera-based context capture) and generational divides in LLM usage further shape deployment.

### *Semantic understanding and knowledge*

Improving agentic AI requires unified access points for scientific data through standardized APIs that agents can call directly—applicable to numerical machine data as well as experimental results. To ground the answers of AI, data should be structured into well-connected knowledge graphs, with digital twins providing test environments for evaluation and benchmarking. Significant challenges include unique facility terminology and non-standard data channel designations; common ontologies are needed to translate everyday language into domain-specific terms. These approaches collectively advance FAIR principles for agentic systems, with AI helping address the human-factors challenge of comprehensive metadata collection.

### *Tools, interfaces and integration*

A clear design direction is emerging: LLMs-as-a-Service architectures providing centralized inference while preserving facility autonomy (e.g., cBORG or the ALCF Inference Service), paired with shared MCP registries for tools and reusable skills. Critical gaps include incomplete documentation, institutional knowledge residing only in individual expertise, difficulty interfacing with legacy systems, and inconsistent metadata capture. As a concrete 12–18 month milestone, the community proposes a cross-facility demonstration where a common agentic workflow operates across multiple sites using facility-specific tools from a shared registry, validating interoperability and portability.

### *Evidence and evaluation*

Demonstrating impact requires robust evaluations beyond anecdotal wins, which occur when broad applicability, correctness, robustness, efficiency, speed, and scalability enable important outcomes consistent with DOE's mission. Agentic systems face particular evaluation challenges: limited coverage of edge cases, incomplete criteria for success, multiple competing objectives, implementation costs (expertise and compute), and time-delayed rewards that make improvement difficult. Breakouts emphasized domain-appropriate benchmarks and conformance tests (especially for cross-facility workflows), plus evidence artifacts that support trust: replayable traces, verified citations, and clear distinctions between retrieved facts and generated content.

## Genesis mission alignment

DOE scientific user facilities underpin research across biology, chemistry, physics, geology, and materials science—including high-priority areas such as critical minerals, quantum information sciences, and energy security. The advances detailed in this report support Genesis science and technology challenges [6] through autonomous workflows enabling complex experiments and high-dimensional search, real-time optimization and control for enhanced user capabilities, integration of DOE user facility datasets, and workforce multiplication spanning literature review to experimental design.

Workshop participants included strong representation from MOAT, SYNAPS-I, and microelectronics seed teams, with direct seed-team discussions in Day 2 breakouts. Representatives from ModCon and AmSC teams provided broader Genesis alignment.

Several cross-cutting activities have DOE-wide and Genesis-wide applicability:

- **Safety-aware agentic systems:** Current accelerator deployments require strict human oversight, safety constraints, and machine protection. These frameworks transfer directly to other Genesis areas with high-consequence failure modes, including modular reactors, electric grid management, and national security applications.
- **Common evaluation and trust frameworks:** Uncertainty quantification, interpretability, and validation/verification are universal needs across Genesis.
- **Standardized tool ecosystems:** User facilities should collaborate with the GM platform pillar to develop ecosystems addressing user-facility-specific requirements.

## Recommendations

***Invest where DOE has a unique competitive advantage***

DOE should prioritize areas where it has unique capabilities that industry cannot readily replicate:

- **Cross-facility coordination infrastructure:** The American Science Cloud, federated agent registries, shared conformance tests, and standardized APIs across national labs represent capabilities no single vendor can deliver. DOE should define and steward an agent-as-user framework—federated identity, interoperable access controls, and auditability—to enable secure cross-site workflows.
- **Safety-critical agentic architectures:** Accelerator and beamline safety constraints—including machine protection systems, personnel safety interlocks, and equipment damage prevention—have produced governance models transferable to other high-consequence domains (e.g., modular reactors, grid management, and national security applications). These patterns represent a DOE contribution with broad applicability.
- **Scale integration:** Integrating DOE-scale datasets, leadership-class HPC resources, and experimental facilities into unified agentic workflows is uniquely enabled by the national lab ecosystem. This end-to-end integration across the scientific lifecycle is difficult to replicate commercially.

***Manage critical risks***

- **Skill atrophy (automation-induced loss of manual expertise):** Automation can erode manual competence; when automated systems fail, recovery becomes slower and riskier. Facilities should treat manual competence as an operational requirement, supported by training and periodic drills.
- **Adoption fragility, turnover, and institutional memory:** Trust can collapse after a single high-profile failure. With 20% annual turnover at some facilities, platforms must remain maintainable without original champions through clear documentation, reproducible deployments, and traceable decision logs. Deployment must also bridge generational differences in LLM adoption through training and demonstrated value, while ensuring quality.
- **10X threshold:** Incremental improvements will not overcome organizational inertia. Only transformative gains (mirror alignment: 1 day → 10 minutes; crystal detection: 98% accuracy) justify adoption costs. Pilots should target high-impact demonstrations, not marginal improvements.

***Address the tacit knowledge problems with improved implementations of FAIR principles***

Across all domains, essential operational expertise remains tacit—held by individual subject matter experts rather than captured in machine-accessible formats. As personnel retire or rotate, this knowledge is at risk of loss, increasing recovery time, training burden, and operational risk.

- **Knowledge graphs and ontologies:** Structured representations linking procedures, equipment states, failure modes, and recovery actions enable agents to reason about operations rather than pattern-match on text.
- **Electronic logbook standardization:** Consistent, searchable logs with structured metadata transform institutional memory from scattered notes into queryable knowledge bases.
- **Observational capture:** Recording expert practices during operations—screen recordings, voice annotations, decision rationales—creates training data for both human successors and AI systems.
- **Agent-assisted templating:** Agents themselves can help improve log quality by prompting operators for missing context and suggesting structured entries based on observed actions.

***Invest in computing and facility infrastructure to realize AI's potential***

Near-term priorities (6–18 months) for enabling safe, scalable deployment:

- **Authentication/authorization frameworks:** Persistent agent identity across facilities with scoped authority, delegation chains, and auditable access logs for long-running cross-site workflows.
- **MCP tool registries:** Shared registries with sandbox environments for testing, versioned tool definitions, and facility-managed LLM inference services that balance capability with security requirements.
- **Digital twins:** Simulation environments for validating agent actions before live deployment—ranging from high-fidelity physics models to "primitive simulations" that capture essential constraints.
- **Metadata capture infrastructure:** The highest-value gap for materials/nanosci-

ence, enabling transformation of context-poor data into ML-ready datasets with complete sample genealogy.
- **Chem/Biosecurity agents:** Automated review and monitoring of user projects against dual-use and safety constraints.
- **Knowledge capture systems:** Tools and workflows to encode tacit SME knowledge in machine-accessible formats before institutional knowledge is lost.

***Partner with industry on general purpose capabilities where they invest***

DOE should partner and leverage external innovation, rather than lead development, in:

- Frontier model development and general-purpose LLM capabilities
- General-purpose agentic frameworks (LangChain, AutoGen)—DOE should adopt and extend, building domain-specific integration layers (e.g., Osprey) or highly scalable backends (e.g., Academy) rather than competing frameworks
- Standard inference infrastructure—incorporate commercial offerings into Lab infrastructure LLMs-as-a-Service where security permits

## Disclosure statement

No potential conflict of interest was reported by the author(s).

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