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Shaping the Future of Self-Driving Autonomous Laboratories Workshop

November 7–8, 2024
Denver, CO, USA

Instruments and Computing across Multi-Domain Networks

AI/ML Integration in Scientific Workflows

Multi-Modal Data Integration

Autonomous Decision-Making in Experiments

User Facility Modernization

Cross-Disciplinary AI/ML Applications

OAK RIDGE National Laboratory

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Table of Contents

Executive Summary

The "Shaping the Future of Self-Driving Autonomous Laboratories" workshop, held in Denver on November 7-8, 2024, brought together leading materials science, chemistry, and computing experts to address the growing need to revolutionize scientific research through AI-driven autonomous laboratories. The workshop explored how recent breakthroughs at the intersection of materials science, chemistry, and computing can accelerate scientific discovery through an ecosystem of interconnected, intelligent research facilities.

The workshop identified several critical challenges in developing autonomous laboratories, including networking heterogeneous platforms of sensors and instruments into complex ecosystems, the integration of data and control messages, the development of AI/ML systems that understand fundamental physical and chemical principles, and the need for comprehensive safety protocols. Participants emphasized the urgent need to address the growing disconnect between human decision-making timescales and modern instrumentation capabilities, as exemplified by experiences at LCLS-II, where data collection rates have outpaced traditional human-driven experimental approaches.

KEY INSIGHTS/RECOMMENDATIONS

- Establish a national consortium for self-driving laboratories that leverages DOE facilities as foundational anchors while integrating academia, industry partners, and other federal agencies to build a sustainable ecosystem for advancing autonomous research and fostering cross-sector innovation.
- Develop software, hardware, digital twin, and networking solutions for sustainable ecosystems with diverse scientific instruments and computing systems across mutli-domain access controls and firewalls.
- Develop hybrid AI systems that combine data-driven learning with fundamental scientific principles, ensuring automated decisions remain grounded in core physical and chemical understanding.
- Address the critical timescale mismatch between human decision-making and modern instrumentation capabilities through strategic automation while preserving essential human insight and oversight.
- Create standardized interfaces and protocols for laboratory equipment and data management to enable seamless integration across facilities and institutions.
- Transform scientific education and workforce development by integrating AI/ML training with traditional scientific curricula while maintaining an emphasis on fundamental principles and critical thinking.

The participants outlined key recommendations for advancing autonomous laboratories, including the development of universal laboratory equipment interfaces, the implementation of automated metadata collection systems powered by AI, and the creation of hybrid AI systems that combine data-driven learning with fundamental scientific principles. Furthermore, the workshop emphasized the critical importance of maintaining human oversight and expertise while leveraging automation, ensuring that human scientific intuition and creativity are preserved and enhanced rather than eliminated.

Education and workforce development emerged as crucial components for success, with participants emphasizing the need to prepare the next generation of scientists for an increasingly automated research environment. The workshop recommended redesigning scientific curricula to integrate AI/ML tools while maintaining a focus on fundamental scientific understanding, developing virtual laboratory environments for hands-on training, and establishing cross-disciplinary programs that combine domain expertise with computational skills while embedding ethical considerations.

The workshop concluded with strong momentum toward establishing a national consortium for self-driving laboratories, with participants emphasizing the need for strategic organization and unified messaging. The proposed consortium would leverage existing DOE facilities as anchors for broader collaboration with academia, industry, and other federal agencies to create a sustainable ecosystem for advancing autonomous laboratory capabilities. Participants noted the importance of demonstrating clear value propositions that address national priorities while ensuring long-term sustainability beyond initial infrastructure funding.

1 Introduction

As we enter a new era of scientific discovery, the global research community faces unprecedented challenges that demand rapid integration of insights across diverse domains. Traditional research methodologies, while historically successful, are increasingly challenged by the complexity and urgency of modern scientific questions. To meet the pressing needs of our time—from climate change to public health to sustainable energy—there is a compelling need to revolutionize our approach to scientific research through the development of smart, interconnected laboratories of the future.

The concept of interconnected scientific facilities represents a transformative opportunity to accelerate discovery through an ecosystem of AI-driven laboratories. Recent breakthroughs combining materials science and high-performance computing (HPC) have yielded tangible results in accelerating scientific discovery, as evidenced by several groundbreaking achievements in the emerging 'Scientific Laboratories of the Future' paradigm [1]. These include the rapid discovery of novel metallic glasses through ML-enhanced high-throughput experimentation [2], the successful isolation of gradient co-polymers using AI workflows in automated chemical synthesis and characterization laboratories [3], the development of new organic semiconductor materials for organic light-emitting diodes or photovoltaics [4], and the accelerated discovery of materials for energy storage and conversion through AI-driven prediction and synthesis of inorganic materials [5]. These achievements, alongside initiatives like ORNL's INTERSECT [6], showcase the synergy between advanced computational methods and materials research, highlighting what is possible when we fully harness the power of artificial intelligence (AI), machine learning (ML), HPC, and autonomous experimentation in a unified research ecosystem.

This inaugural workshop brought together leading experts from materials science and computing to explore the vision of 'Scientific Laboratories of the Future' and chart a course for their implementation. We examined how the convergence of these fields enables key technological elements required for this transformation—from interoperable facility ecosystems and AI agents to autonomous synthesis platforms and secure data infrastructure—while addressing the challenges and opportunities in creating a scalable, intelligent research environment. Through this interdisciplinary collaborative effort, we aim to define the roadmap for a research infrastructure that can accelerate scientific discovery at an unprecedented pace and scale, enabling us to address some of humanity's most pressing challenges.

Workshop Structure. The two-day workshop, held on November 7-8, 2024, was structured to facilitate comprehensive discussions on shaping autonomous laboratories of the future. The first day began with introductory sessions, followed by two series of short talks featuring speakers from various institutions, including ORNL, CMU, NCSU, JHU / PNNL, and UTK. Interactive breakout sessions complemented these presentations with focused discussion on examining current challenges, state-of-the-art developments, and both short- and long-term goals. The second day featured a panel discussion on "Integrating Traditional Scientific Methods with AI/ML-Driven Autonomous Laboratories," with experts from SLAC, PNNL, ORNL, and Sandia. The workshop addressed key topics including AI/ML integration in scientific workflows [7, 8, 9, 10], multi-modal data integration, autonomous instrument control and real-time decision-making in experiments [11, 12], user facility modernization, digital twins of data-driven computational modeling and emulation of scientific ecosystem infrastructure [13, 12], and cross-disciplinary AI/ML applications. The discussions also emphasized the critical role of reproducibility in scientific workflows [14] and scalable data analysis frameworks [15], efforts to enable end-to-end reproducible and FAIR (Findable, Accessible, Interoperable, and Reusable) data analysis and provenance [16, 17, 18], and unique challenges for autonomous laboratories in synthetic biology [19]. Throughout both days, dedicated breakout sessions and working lunches provided opportunities for in-depth discussions and collaborative development of the workshop report, ensuring a balanced approach to exploring both technical challenges and practical implementation strategies for autonomous laboratories.

2 Interactive Breakout Sessions

The workshop convened breakout sessions to address critical challenges in developing and implementing autonomous laboratories. The sessions focused on five key areas: AI/ML integration in scientific workflows, multi-modal data integration, autonomous decision-making in experiments, user facility modernization, and cross-disciplinary AI/ML applications. Participants were charged with addressing four fundamental questions: how to effectively integrate heterogeneous data from multiple sources into AI-driven autonomous workflows; what challenges exist in developing AI/ML systems that understand underlying physical and chemical principles; how to prepare the next generation of scientists to leverage AI/ML tools; and what ethical considerations and safeguards should be established for autonomous scientific research. Through these discussions, participants aimed to establish both short-term goals for immediate implementation and long-term strategic objectives for advancing the field of autonomous laboratories.

2.1 Instrumentation and Ecosystem Integration

The discussions revealed a complex landscape of automating scientific workflows that span a wide variety of instruments (e.g., microscopes, 3D printers, chemical sythesizers, flow reactors, and electrodeposition machines) and computing platforms (e.g., edges, clouds, clusters, and supercomputers) [20]. The instruments range from established industry products to those not designed for networking or automation that present unique integration challenges in science environments. Companies such as Emerald Cloud Lab, Siemens, GE/Fanuc, AllenBradly, and Automationdirect offer a sophisticated ecosystem with hardware and software infrastructure capabilities. However, several scientific workflows — for example, catalyst characterization applications, material property analysis, plant monitoring, and other niche resources — require custom instruments such as pumps, syringes, and soil monitors [21]. These workflows are typically executed in closed-loop, where measurements are streamed to HPC systems, and the resultant decisions are sent back for updating parameters to repeat the experiments. However, the heterogeneity and deployability of the instruments pose challenges in fine-grained design for orchestration and control of autonomous and high-throughput experiments across multi-domain networks with stringent firewalls and access controls.

An ecosystem for automated, multi-domain scientific workflow requires robust infrastructure design to network the instrument systems (custom devices, storage, control hardware, and software platforms) with other computing and storage resources across the ecosystem [12]. Specifically, they should enable effective workflow orchestration across complex firewalls and access controls across multi-domain networks.

The integration of scientific instruments into the ecosystem should provide seamless instrument control and data management (e.g., acquisition, transferring, and processing), in particular across multi-vendor instruments. Most scientific experiments are orchestrated locally, where instruments are controlled via propitiatory GUIs or possibly by limited capability APIs. Here, measurements are collected manually from different instruments and processed differently prior to integration into workflows. This becomes a multifaceted challenge, where the complexity of handling various data types and file formats affects providing an abstracted agnostic data interface integrated to scientific workflows. Hence, Participants emphasized that accessible and seamless interfaces for instrument control, and data collection and management, are essential for remotely orchestrating autonomous workflows and steering self-driven laboratories, particularly when real-time decision-making is required.

Digital twins have been extensively discussed as a promising solution for the testing and development of autonomous systems [22]. They can effectively mirror physical beamline setups, complete with web-based visualization and sensor readings, as demonstrated by ILL France DAQ. Digital twins can also emulate ecosystem infrastructure to enable the development of distributed workflows and instrument control plane [23, 24]. This approach enables both low-accuracy interface testing for development purposes and high-accuracy physics simulations for experimental planning. Participants noted that such digital twins could serve multiple purposes [25]: training users, testing control systems, developing distributed workflows, and providing a safe environment for developing autonomous workflows. However, they also acknowledged the significant computational resources required to maintain accurate real-time digital twins and the challenge of keeping these digital representations synchronized with their physical counterparts.

Insights/Recommendations:

- Develop network and software solutions for orchestrating instruments, and computations across diverse domains protected by firewalls and access policies.
- Create standardized interfaces and control protocols for laboratory equipment to ensure effortless integration across various manufacturers and systems.
- Develop a standardized middleware interface to integrate proprietary control systems, facilitating unified laboratory automation without needing alterations to manufacturers' existing systems.
- Develop adaptable modular digital twin frameworks capable of accurately simulating equipment behavior and experimental processes for testing and validation.

2.2 Data Management and Standardization

Data and metadata management has emerged as a critical challenge in the development of autonomous laboratories. The discussion highlighted the need for data capture to extend beyond mere experimental results, incorporating environmental factors, equipment conditions, operator activities, and minor variables that could impact outcomes. Participants cited experiences where unforeseen variables notably influenced results, underscoring the importance of systems capable of recording both evident and subtle experimental influences. They noted that comprehensive data collection is essential for replicating experiments and facilitating effective AI-driven decision-making.

Existing data management models, such as materialscommons.org and the Protein Data Bank (PDB) [26], were extensively analyzed as potential templates for a wider implementation. These systems demonstrate the value of domain-specific approaches to data organization and access, but participants noted that they also reveal the challenges of scaling such solutions across different scientific domains. The discussions led to proposals for creating more flexible and adaptable data collection and management systems that could accommodate diverse scientific fields while maintaining standardization where possible. Participants emphasized the need for systems that could evolve as new types of data and experimental methods emerge.

The quality and validation of data emerged as a critical concern, with participants sharing experiences of how "bad" or "imbalanced" data can impact research outcomes. The current practice of treating all data equally in many systems was identified as a significant problem. The group proposed developing sophisticated data qualification mechanisms that could automatically assess data quality based on multiple parameters and experimental conditions. This would include systems to detect potential problems, track data provenance, and maintain detailed records of experimental conditions that could affect data quality. The discussions also touched on the challenge of maintaining data integrity while allowing for necessary corrections and updates.

The development of automated tools for metadata collection was identified as crucial for enabling effective cross-facility work. The group explored how domain-specific Large Language Models (LLMs) could be employed to intelligently interpret and integrate external information with experimental data. These systems would need to understand complex scientific contexts and be able to extract relevant information from various sources, including laboratory notebooks, equipment logs, and environmental monitoring systems. Participants emphasized that such tools would need to balance automation with human oversight to ensure the accuracy and reliability of the collected metadata.

Insights/Recommendations:

- Design adaptable domain-specific data standards and ontologies that progress with scientific advances while ensuring interoperability.
- Implement AI-driven automated systems for metadata collection to efficiently capture detailed experimental contexts and data provenance without adding to researchers' workload.
- Establish incentive mechanisms and create technical frameworks for high-quality data sharing across institutions, similar to successful examples such as the Protein Data Bank.

2.3 AI/ML Implementation and Autonomous Decision-Making

The workshop participants engaged in extensive discussions about the fundamental challenges of developing AI/ML systems capable of understanding and optimizing for the underlying physical and chemical principles. For example, a cutting-edge AI/ML model can be developed and implemented to verify the sanity of the geometric shape of a flow reaction in real time of an electrochemistry workflow performed at the ORNL Autonomous Chemistry Laboratory (ACL) [9] and convert digital twin measurements to match physical networks [27]. Unlike traditional parameter optimization, these systems need to grasp complex scientific relationships and make decisions based on fundamental principles. The participants emphasized that current AI systems often excel in finding patterns in the data but struggle to incorporate a theoretical understanding of physical and chemical processes. This limitation becomes particularly apparent when systems encounter conditions outside their training data, highlighting the need for AI architectures that can combine empirical data with theoretical and physical knowledge [28].

The challenge of training models to identify research gaps and opportunities emerged as a crucial topic. Participants discussed the need for comprehensive schemas and reference databases that could serve as benchmarks for identifying missing information. They emphasized that these systems need to go beyond simple pattern recognition to identify potentially valuable research directions that have not been explored. This requires developing AI systems that can understand the significance of gaps in scientific knowledge and prioritize experiments that could fill these gaps. The group also discussed the importance of developing systems that can recognize when unexpected results might indicate promising new research directions rather than experimental errors.

Foundation models have recently garnered considerable attention as a transformative force in scientific research [29, 30, 31]. Participants noted that major technology companies like Google and Meta are developing foundation models for materials research, particularly in pharmaceuticals, but expressed concern that these models often remain proprietary and inaccessible to academic researchers. The group emphasized the need for open and accessible foundation models that could serve the broader scientific community. They discussed strategies for developing such models, including the challenges of aggregating diverse scientific data sources and the computational resources required to train these large-scale models.

The integration of real-time decision-making capabilities emerged as a critical requirement for autonomous laboratories [11, 32]. Participants discussed the challenges of developing systems that can process multi-modal data streams in near real-time and make informed decisions about experimental parameters. They emphasized the need for systems that can balance multiple objectives, such as maximizing experimental throughput while maintaining safety and data quality. The group also explored the potential of digital twins for near real-time experiment monitoring and control, although they noted the significant computational challenges involved in maintaining accurate near real-time simulations.

Insights/Recommendations:

- Develop hybrid AI models that integrate data-driven learning with core physical and chemical principles to ensure scientifically valid decisions.
- Establish benchmark datasets and validation frameworks specifically for evaluating scientific AI systems' ability to understand underlying principles.
- Create open-source foundation models for scientific research to prevent dependence on proprietary commercial systems.

2.4 Education and Workforce Development

To meet the changing dynamics of scientific research, it is crucial to redesign educational and training frameworks, enabling future scientists to effectively incorporate AI/ML into the scientific method. Participants engaged in detailed discussions on how to prepare the next generation of scientists for a research environment increasingly dominated by AI/ML tools. They emphasized that preparation must go beyond simply teaching programming or data science skills to include a deep understanding of how AI/ML tools and the underlying mathematical principles can be integrated into the scientific method. Current educational programs often treat AI/ML as an add-on rather than an integral part of scientific curriculum and training, creating a gap between traditional scientific education and the skills needed for modern research. Participants proposed developing new curricula that would strengthen mathematical foundations while making advanced concepts more accessible through practical applications. A crucial aspect is the development of new educational resources with hands-on examples that integrate different scientific disciplines, experimental design principles incorporating AI/ML tools, and provide the foundations to learners of diverse backgrounds [33].

Encouraging the next generation of scientists to embrace automation and AI/ML tools is one side of the coin, as our community reliance on such tools can be detrimental to developing strong fundamental knowledge. Automation and AI/ML tools have the potential to become a "closed box" that students rely on without understanding the underlying physical and abstract principles. Therefore, it is necessary to strike a balance between automation and core scientific comprehension. Strategies were discussed to ensure students develop strong foundational knowledge while learning to leverage advanced computational tools. This included proposals for new educational approaches that would integrate theoretical understanding with physical and abstract laws of science domains [34], ensuring students can critically evaluate the outputs of AI systems and understand their limitations [28].

The need for comprehensive mathematical training across scientific disciplines was emphasized as Participants noted that many scientists lack the mathematical background necessary to fully understand and incorporate AI/ML tools in scientific research. They proposed developing new curricula that would strengthen mathematical foundations while making advanced concepts more accessible through practical, hands-on applications. The group also discussed the importance of teaching experimental design principles that incorporate AI / ML tools, ensuring that students understand how to design experiments that can effectively utilize these technologies.

Interdisciplinary education became a central focus, with participants highlighting that scientists should grasp not only their specialized area but also the computational and ethical dimensions of their research. They discussed the development of training programs that would combine technical skills with broader considerations about the impact of autonomous research systems. This included proposals for incorporating ethics training, data management principles, and communication skills into scientific education and developing hands-on training opportunities with autonomous laboratory systems, possibly through virtual labs and simulators.

Insights/Recommendations:

- Revamp scientific curricula to incorporate AI/ML tools while maintaining the emphasis on core scientific principles and analytical skills.
- Create virtual laboratories that allow students to safely engage with autonomous systems for practical hands-on experience.
- Establish cross-disciplinary training programs that combine domain knowledge with computational skills and ethical considerations.

2.5 Ethics and Safety Considerations

The ethical considerations related to autonomous research systems have generated significant discussions concerning safety protocols and responsible usage. Participants highlighted that autonomous systems handling hazardous materials or dangerous equipment require multiple layers of safety procedures and careful consideration of failure modes. This requires comprehensive safety protocols that account for both routine operations and emergency situations, including the development of fail-safe mechanisms that safely shut down experiments if anomalous conditions are detected. This highlights the importance of maintaining human oversight for critical safety decisions, even in otherwise autonomous systems.

The debate over suitable automation levels in autonomous systems centers on the necessity of human supervision for various decision types. Participants worked to develop frameworks for determining which decisions could be safely automated and which required human input. Maintaining human expertise, scientific intuition, and creativity is crucial as research environments become more autonomous, ensuring that scientists retain the ability to understand and intervene in automated processes when necessary.

Data ethics emerged as a complex challenge requiring careful balance between open science principles and practical considerations. Participants engaged in detailed discussions on proper attribution of data contributions, the challenges of maintaining data privacy when required, and the need for clear protocols regarding data sharing and reuse. They explored various models to encourage data sharing while protecting intellectual property rights, including proposals for new types of scientific credit that would recognize valuable dataset contributions. The group also discussed the challenges of ensuring data quality and preventing the propagation of incorrect or misleading data through automated systems.

Responsible innovation in the creation of autonomous laboratories has generated considerable interest. Participants discussed the need for proactive approaches to identifying and mitigating potential risks, including the use of adversarial AI systems to identify potential failure modes, dangerous experimental conditions, or malicious intent. They emphasized the importance of developing robust validation and verification methods for both experimental and computational approaches, ensuring that autonomous systems make reliable and safe decisions. The group also explored the broader societal implications of autonomous laboratories, including their potential impact on the scientific workforce and the accessibility of scientific research.

Insights/Recommendations:

- Establish multi-tiered safety systems with well-defined protocols for human supervision over crucial autonomous laboratory decisions.
- Implement robust, comprehensive frameworks to ensure data quality, attribution, and sharing that protect intellectual property while promoting open science.
- Develop advanced risk evaluation tools, incorporating adversarial AI methods, to preemptively detect safety risks in physical labs.

3 Panel: Integrating Traditional Scientific Methods with AI/ML-Driven Autonomous Laboratories

Leading scientists from four major national laboratories gathered for a critical discussion on revolutionizing laboratory research, as Ryan Coffee (SLAC), Vijay Murugesan (PNNL), Marshall McDonnell (ORNL), Dale Huber (SANDIA), and moderator Rafael Ferreira da Silva (ORNL) examined how to seamlessly merge traditional scientific approaches with AI and ML technologies in experimental settings. The panel aimed to address how the scientific community can create truly autonomous laboratories while maintaining scientific rigor and preserving valuable human insight. With a focus on practical challenges and opportunities, the discussion sought to identify pathways for leveraging AI/ML capabilities to accelerate scientific discovery while ensuring that these advanced technologies complement rather than replace human scientific intuition. This timely conversation was particularly relevant given the increasing sophistication of scientific instrumentation and the unprecedented volumes of data being generated in modern research facilities.

Discussion. The panel discussion opened with a critical examination of the growing disconnect between human and machine operational timescales in modern scientific facilities. This challenge was powerfully illustrated through a recent experience at the Linac Coherent Light Source (LCLS-II) [35], where the data collection rate has become so rapid that traditional human-driven experimental approaches are becoming a bottleneck. While human operators typically require minutes to adjust experimental parameters, the facility can now generate what would previously have been an hour's worth of data in just 30 seconds, highlighting a fundamental mismatch between human decision-making speeds and advanced scientific instrumentation capabilities.

The discussion revealed a key tension between the urgent push for automation and the necessity to uphold scientific rigor and prevent errors. Panelists noted that given the rapid data collection rates in modern facilities, automation is unavoidable. However, there is a substantial risk of compromising traditional and rigorous experimental methodologies if automation is implemented hastily. Therefore, facilities face a complex challenge in balancing the demand for speed with maintaining the integrity of experiments.

The discussion also emphasized the importance of documenting the transition period between conventional and autonomous experimentation. The panelists stressed that this current interface period presents a crucial opportunity to capture and preserve human insight and intuition before fully autonomous systems become widespread. This documentation process is seen as essential for ensuring that future automated systems can incorporate the valuable human expertise and experimental wisdom that has been developed over years of traditional scientific practice.

A significant portion of the discussion focused on the need to carefully integrate human insight with automated systems rather than simply replacing human decision-making entirely. Panelists noted that successful integration of AI/ML technologies in scientific facilities will require thoughtful consideration of where human intuition and creativity are most valuable and how these qualities can be preserved and enhanced through automation rather than eliminated.

Looking ahead, the panel outlined essential actions for a successful transition, including detailed documentation of current experimental processes, identifying critical areas requiring human insight, designing adaptable automated systems for various scientific fields, and setting defined standards for validating autonomous experiment results. The consensus favored a hybrid approach, integrating AI/ML for speed and efficiency while maintaining essential human insight and strict experimental methods.

Insights/Recommendations:

- Scientific institutions urgently need to resolve the disparity between human decision-making speeds and the capabilities of modern instruments to avoid workflow bottlenecks.
- The present transition period offers a crucial and unique window for documenting human expertise and experimental wisdom before fully autonomous systems become widespread.
- Although automation is unavoidable, accelerating its adoption without understanding traditional methods can lead to systematic errors, potentially affecting the quality of research.
- Research facilities need strategic hybrid approaches that preserve human insight and creativity while leveraging AI/ML capabilities for enhanced experimental efficiency.

4 Building a National Labs of the Future Consortium

The workshop concluded with strong momentum toward the establishment of a continuing workshop series aimed at building a national consortium for self-driving laboratories. Participants noted that this initial workshop, which combined materials science with computational aspects, served as a crucial first step in bringing together diverse stakeholders to advance this initiative. They stressed the urgency of immediate action, recognizing that typical funding cycles leave the community with a narrow window of approximately three years to showcase tangible results and secure long-term support for the consortium's mission.

A critical focus of the discussion was the need for unified messaging and strategic organization. Participants emphasized that the next workshop should address several pressing topics, including organizational structure, mapping of industry partners and instrument manufacturers, and the role of computing research. They stressed the importance of bringing in the right industry partners—those who understand collaborative approaches rather than purely commercial interests—and suggested documenting potential partners in their shared online document. The group also discussed the potential for hackathons to foster collaboration between teams and innovate solutions to pressing challenges, with a possible first event proposed for early 2025.

The discussion highlighted the strategic importance of positioning the consortium in relation to existing government programs and initiatives. Rather than trying to create entirely new structures, participants suggested demonstrating how the consortium could enhance and harness existing capabilities and infrastructure. They emphasized the need to clearly articulate the value proposition, particularly in addressing national priorities through the leveraging of user facilities. The group noted that having compelling examples of how self-driving laboratories could serve national interests would be crucial for gaining support, including from

Congress.

The sustainability of the initiative was also a pivotal topic of discussion. Participants emphasized that while initial infrastructure development would need funding, long-term vision prioritizes creating self-sustaining smart laboratories. They discussed how this could work in practice, with DOE facilities potentially serving as anchors for broader collaboration with academia and industry. The group noted the importance of developing capabilities that would allow various stakeholders, including academic institutions, to effectively interact with and utilize DOE resources as part of their research efforts. This approach would help create an integrated ecosystem where resources and expertise could be shared effectively across the consortium.

Insights/Recommendations:

- Establish a sustainable consortium structure through strategic workshops and hackathons that bring together DOE facilities, academia, and industry partners to advance self-driving laboratories.
- Develop a cohesive platform that illustrates how the consortium bolsters current capabilities and aligns with national priorities, without establishing entirely new frameworks.
- Create a compelling value proposition that harnesses DOE resources and facilities while enabling broad collaboration across institutions to ensure long-term sustainability beyond initial infrastructure funding.

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Appendix A: Participants and Contributors

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Appendix B: Agenda

Day 1 – November 7, 2024	
9:00-9:20am MST	**Welcome and Introductions** *Rafael Ferreira da Silva (ORNL), Ben Mintz (ORNL)*
9:20-9:40am MST	**Overview of the Workshop Organization, Goals, and Charge Questions** *Rafael Ferreira da Silva (ORNL)*
9:40-10:40am MST	**Short Talks (Session 1)** • Talk 1: Ben Mintz (ORNL) • Talk 2: Theresa Mayer (CMU) • Talk 3: Martin Seifrid (NCSU)
10:40-11:00am MST	*Break*
11:00am-noon MST	**Short Talks (Session 2)** • Talk 4: Mitra Taheri (JHU/PNNL) • Talk 5: Michela Taufer (UTK) • Talk 6: Nagi Nageswara (ORNL)
noon-1:30pm MST	*Working Lunch (discussions with short-talk presenters)*
1:30-3:00pm	**Breakouts session:** challenges and state-of-the-art
3:00-3:30pm MST	*Break*
3:30-4:30pm	**Breakouts session:** short- and long-term goals
4:30-5:00pm MST	**Summary of breakouts discussions**

Day 2 – November 8, 2024	
9:00-9:15am MST	**Summary and Highlights of Day 1** *Rafael Ferreira da Silva (ORNL)*
9:15-10:00am MST	Panel: **Integrating Traditional Scientific Methods with AI/ML-Driven Autonomous Laboratories** • Moderator: Rafael Ferreira da Silva (ORNL) • Panelists: Ryan Coffee (SLAC), Vijay Murugesan (PPNL), Marshall McDonnell (ORNL), Dale Huber (Sandia)
10:00-10:30am MST	*Break*
10:30-noon	**Breakouts session:** Drafting the Workshop Report (bullet points)
noon-1:00pm MST	*Working Lunch (discussions with short-talk presenters)*
1:00-2:00pm MST	Topics for next workshops and final discussions
2:00-3:00pm MST	Collaborative meetings (optional)