
INNOVATION X LAB℠
ARTIFICIAL INTELLIGENCE SUMMIT
October 2–3, 2019 × CHICAGO

INNOVATION X LAB℠

Welcome.

InnovationXLab: Artificial Intelligence Summit, hosted by Argonne National Laboratory, is the fourth in the U.S. Department of Energy's (DOE) InnovationXLab series — a showcase of the remarkable assets and capabilities of the Department's National Laboratories. These summits facilitate a two-way exchange of information and ideas between industry, universities, investors, and end-use customers with Lab innovators and experts.

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Welcome to Chicago—America's Second City! With more than 100 neighborhoods, eight major-league sports teams, a thriving arts and theater culture, and a fast-growing technology hub, Chicago is both a great place to live and to work.

The Chicagoland area is also home to two of the U.S. Department of Energy's (DOE) 17 National Laboratories: Argonne National Laboratory—your host for today's event—and Fermi National Accelerator Laboratory, enriching the region with some of America's top science talent and attracting researchers and businesses from around the globe to our user facilities.

American leadership in Artificial Intelligence (AI) is critical to driving innovation and maintaining our nation's economic competitiveness and security. DOE established its Artificial Intelligence and Technology Office (AITO) to harness and accelerate the Department's preeminent leadership in high-performance computing, facilities, and team science in applying AI across the entire National Laboratory system—to increase the pace of discovery in energy, materials science, health care, transportation, and beyond.

DOE laboratories house four of the ten fastest and most powerful supercomputers in the world, uniquely positioning DOE to redefine what is possible in AI. Under the leadership of Energy Secretary Rick Perry, the Department has gone all-in on this emergent field. We are in the midst of the Golden Age of AI, and DOE's world-class scientific and computing capabilities will be critical to securing America's AI dominance.

Innovation*X*Lab℠: Artificial Intelligence Summit is the fourth in DOE's Innovation*X*Lab series — a showcase of the assets and capabilities of the Department's National Laboratories. Over the next two days, you will hear from some of the nation's brightest minds in AI, with ample opportunities to network, make connections, and jump-start conversations with National Lab innovators and experts. It is our hope that these new relationships will be the start of a new era of American leadership in AI. Thank you for joining us.

Enjoy the Summit!

Paul K. Kearns, Ph.D.

Director
Argonne National Laboratory

Conner Prochaska

Chief Commercialization Officer
and Director
Office of Technology Transitions
U.S. Department of Energy

Artificial Intelligence at the U.S. Department of Energy

Today, U.S. Department of Energy (DOE) National Laboratories house four of the ten fastest and most powerful supercomputers in the world, uniquely positioning DOE to push the limits of artificial intelligence (AI) and to accelerate the pace of discovery in a wide variety of areas.

DOE's Artificial Intelligence Program (DOE AI) was established to harness the Department's world-class leadership in high-performance computing, facilities, and team science to build upon and accelerate America's existing AI research in all of these areas and more.

ENERGY

- Multiple DOE labs are using AI technologies and tools to prevent, detect, and effectively respond to electric grid disruptions, strengthening the resiliency of our grid.
- Idaho National Lab researchers are also using AI to discover better ways to turn organic matter into energy.
- Argonne National Laboratory researchers are developing new ways to extract insights from vast quantities of data on the electric grid using AI, enabling greater reliability, resilience, and efficiency.
- Sandia National Laboratories researchers are using machine learning (ML) to reduce the computational cost of computing systems and save energy.
- National Energy Technology Lab is expanding its work to develop the next generation of methane leak detection technology, using an AI aerial platform. The lab is also collaborating with several other labs to develop next-generation, extreme-environment materials for use in advanced fossil energy power systems.
- Brookhaven National Laboratory scientists have developed new AI methods to accurately predict solar energy yield, enabling easier integration of renewable energy into the power grid.
- Brookhaven Lab also is developing a new analysis on the wire AI infrastructure to evaluate and predict energy demands more accurately while data are streaming in the network, affording near-real/real-time load forecasting and state estimation capabilities.
- Researchers at the Princeton Plasma Physics Laboratory are using AI to rapidly predict plasma disruptions that can halt fusion reactions and damage the magnetic devices that house them. Researchers also are applying AI to train models for real-time control of plasma behavior so that fusion energy can become a reality.
- Ames Laboratory is working with the National Energy Technology Lab on projects that demonstrate how several AI-based techniques can be applied to improve power plant performance.
- Oak Ridge National Laboratory researchers are using AI to reliably monitor the performance of nuclear power plants and make adjustments in real time far more efficiently and without human error.
- DOE is also supporting an effort to achieve higher efficiency coal plants using AI techniques.

NATIONAL SECURITY AND EMERGENCY RESPONSE

- Scientists are using AI to better understand research that could help assure the safety, security, and effectiveness of the U.S. nuclear deterrent. Researchers at Pacific Northwest National Lab are using AI to strengthen nuclear non-proliferation by testing signals of potential significance.
- Idaho National Lab has developed an autonomic intelligent cyber sensor, which gives industries the power to quickly identify and divert hackers, using machine learning to identify and map industrial control systems.
- Sandia Labs is using synthetic data generated from nuclear war games to enhance current decision-making processes and aid in identifying complex crisis de-escalation strategies.

- SLAC National Accelerator Laboratory and Berkeley Lab are using AI to prevent or minimize electric grid failures and bounce back faster from storms, solar eclipses, cyberattacks, and other disruptions. Los Alamos Lab is analyzing massive amounts of seismic data to help them better understand earthquakes, anticipate how they will behave, and provide quicker and more accurate early warnings.
- Oak Ridge National Laboratory tools can monitor thousands of events per second to detect anomalies that would escape human analysts by providing network operators with smaller amounts of data that are easier to manage and review. This capability allows them to investigate potential threats and make more informed decisions.

MATERIALS SCIENCE

- Ames Laboratory is using AI methods to speed up the materials discovery process by screening tens of thousands of potential systems to a handful of promising combinations of highly abundant elements for novel compounds that could radically improve the energy efficiency of refrigeration technologies.
- Scientists at Fermilab are using machine learning to search for discovery science and to develop a deeper understanding of fundamental forces and particles, such as neutrinos.
- SLAC researchers are using AI and accelerated experiments to speed the discovery of metallic glasses, materials that are stronger and more efficient than today's best steel, at a fraction of the time and cost required for conventional discoveries.
- Sandia Labs researchers are using deep learning to discover material anomalies in seconds that would take human eyes hours to find.
- Berkeley Lab researchers are developing generative machine learning models that can discover new scientific knowledge about molecular interactions and structure-function relationships in the chemical sciences.
- Brookhaven Lab researchers have developed new streaming AI data analysis methods to help control the investigation and optimization of industrial catalysts in real time during experiments at the National Synchrotron Light Source II.
- Oak Ridge National Laboratory researchers are using AI to dramatically accelerate understanding of material behavior at the atomic level, increasing the efficiency of battery materials and enabling the discovery of new processes and materials to advance battery technology.

MANUFACTURING

- Argonne researchers are using machine learning, a form of AI, to help companies slash engineering design time and cost. Product development that once took months now can be completed in days.
- Machine learning work by Argonne researchers is providing a clearer picture of advanced manufacturing processes, thus making them more efficient and effective.
- Researchers at Fermilab are developing smart sensors and advanced software for "real-time" (nanosecond scale) AI.
- The control of complex systems with AI, for example particle accelerators and telescopes, is an area of research at Fermilab with implications for industrial control and intelligent facilities.
- Berkeley Lab researchers are using generative adversarial networks for the creation of fast, inexpensive surrogate models to allow them to quickly explore a wide parameter design space in combustion.
- Using AI image processing techniques developed at Oak Ridge National Laboratory, researchers can inspect parts in real time throughout the manufacturing process to locate cracks and other quality defects, reducing costs and time to market.

HEALTH CARE

- Argonne, Los Alamos, Lawrence Livermore, and Oak Ridge Lab scientists are using AI and ML to develop new approaches to predicting and treating cancers as part of the CANDLE (CANcer Distributed Learning Environment) consortium.
- Researchers at Sandia Labs are employing deep learning methods to discover DNA regulatory motifs that are important for advancements in medical treatment and understanding of cell processes.
- Researchers are using AI to create more accurate representations of pathology reports and interpretations of mammograms and to improve vaccination campaigns, diagnoses, treatments, and outcomes for Americans, from children to veterans.
- Scientists at Lawrence Livermore, Berkeley, and Argonne Labs are using AI and DOE's supercomputing capabilities to improve understanding of, and develop better treatments for, traumatic brain injuries.
- Scientists at Berkeley Lab are using ML-powered toolchains capable of aiding human researchers in the exploration, sub-setting, and narrowing of health data to better enable suicide prevention.
- Brookhaven National Laboratory has developed groundbreaking AI methods to predict early-onset Alzheimer's and disease progression, paving the way for new preventative treatments to increase patient quality of life.
- Researchers at Oak Ridge National Laboratory are running machine learning algorithms on the lab's Summit supercomputer to scan millions of medical documents in search of relationships that could uncover which factors are responsible for the development of certain diseases.

TRANSPORTATION

- Researchers at Argonne, Oak Ridge, and Sandia Labs are using AI and ML to address complex transportation problems, including reducing traffic jams, improving fuel efficiency, and predicting how transportation will evolve in the future.
- Researchers at Berkeley Lab have launched projects to apply AI to self-driving cars in order to smooth traffic, reduce fuel consumption, and improve air quality predictions.
- Researchers at Sandia Labs developed Whetstone, an open-sourced software application that trains conventional artificial neural networks to behave like spiking neural networks, paving the way for high-powered computing in size-, weight-, and power-restricted environments.
- Scientists at Berkeley Lab are using ML on more than 11,000 infrastructure sensors (inductive loops in highway) to predict traffic dynamics one hour into the future. They are now exploring using the same machine learning model on mobile device data to see if they can reduce the reliance on embedded sensors.
- Oak Ridge National Laboratory geospatial scientists are using advanced machine learning methods to better predict home-to-work commuting patterns to reduce traffic and pollution and drive infrastructure choices.

INNOVATION X LAB℠

Exhibitors

Partnership and Commercialization officers with the DOE National Lab exhibitors are on hand to discuss opportunities to engage and access Lab facilities, technologies, and expertise — **and help bridge the gap between research and commercialization.**

Ames Laboratory

Ames Laboratory is a government-owned, contractor-operated national laboratory of the U.S. Department of Energy (DOE), operated by and located on the campus of Iowa State University in Ames, Iowa. With its roots in the Manhattan Project, Ames Laboratory specializes in materials design, synthesis and processing; analytical instrumentation design and development; materials characterization; catalysis; computational chemistry; condensed matter theory; and computational materials science and materials theory.

CALORIC COOLING

Ames Laboratory leads an effort to design, discover, and deploy new materials that can create temperature changes — caloric effects — for advanced, solid-state refrigeration. The goal is to save up to 30 percent in energy usage in new refrigerators. Ames Laboratory's team integrates AI methods to speed up the materials discovery process by screening tens of thousands of potential systems that could be engineered to generate cooling when acted upon by magnetic, electric or mechanical forces.

This AI-assisted screening produced a handful of promising combinations of highly-abundant elements that were used to prepare and characterize a number of novel compounds that exhibit the best caloric effects known today. Ames Laboratory welcomes participation of industry partners interested in employing these new materials in next-generation, highly-efficient, solid-state caloric-cooling devices.

POWER PLANT PERFORMANCE

Ames Lab is working with the National Energy Technology Laboratory (NETL) on three projects that demonstrate how several AI-based techniques can be applied to improve power plant performance. The techniques developed for these projects were tested in a 100 kW laboratory-scale gas turbine power system. One project demonstrates that supervised and unsupervised machine learning techniques can provide early prediction of surge and stall. A second project shows that a monitoring tool based on an empirical model (developed by Ames Laboratory and NETL) running parallel to a physical power plant is able to predict dynamic operation and detect performance drifting due to potential deterioration. In the third project, an agent-based control algorithm was developed to manage the dynamic coupling of advanced energy systems.

CONTACTS

Julienne Krennrich
jmkrenn@ameslab.gov

Mark Bryden
kmbryden@iastate.edu

Argonne National Laboratory

Argonne's goal in the AI space is ambitious: establish global leadership in the development of AI for science. Our goal will be enabled by the capabilities of the Aurora exascale system scheduled to begin conducting science at Argonne in 2021; a solid strategic plan and the world-class expertise to carry it out; and partnerships with industry, academia, and other national laboratories across the DOE complex.

As AI methods transform how scientists approach both basic and applied research — expanding the boundaries of science and accelerating the rate of discovery — researchers at Argonne are developing machine learning methods, software tools, infrastructure, hardware, and architecture to speed the AI revolution. We are applying these new technologies and methods to key science and engineering research important to DOE and the nation: predicting and treating cancer, developing better treatments for traumatic brain injuries, optimizing superconductors, improving material properties, and addressing complex transportation problems, among many others.

We are training deep neural networks to design better materials and interpret images, simulate molecular behavior, and determine atomic structure on the fly in X-ray and electron microscopy analysis. We are exploring opportunities to use AI approaches in cosmic microwave background experiments, solving classification, estimation, and statistical inverse problems in cosmology and recognizing patterns in particle detectors. We are exploring AI hardware capable of providing the raw computing power needed for AI applications and investigating how new architectures can support big data and computing at the "edge."

In 10 years, we anticipate that learned models will begin to replace data, experimental discovery will be dramatically faster and more accurate, simulation and AI approaches will merge, and AI will be an integral part of scientific discovery. Come visit our booth to explore how you can partner with us in our AI for Science endeavor, leveraging our unique mix of the country's foremost high-performance computers and world-leading scientific expertise.

Argonne National Laboratory seeks solutions to pressing national problems in science and technology. The nation's first national laboratory, Argonne conducts leading-edge basic and applied scientific research in virtually every scientific discipline. Argonne researchers work closely with researchers from hundreds of companies, universities, and federal, state and municipal agencies to help them solve their specific problems, advance America's scientific leadership and prepare the nation for a better future. With employees from more than 60 nations, Argonne is managed by UChicago Argonne, LLC for the U.S. Department of Energy's Office of Science.

CONTACTS

Paulina Rychenkova
prychenkova@anl.gov

John Harvey
harveyj@anl.gov

Brookhaven National Laboratory

Brookhaven National Laboratory (BNL) is a 5,000-acre multipurpose research institution located east of New York City in central Long Island, N.Y. With its diverse, world-class scientific expertise and capabilities, Brookhaven Lab advances discovery and innovation at the frontiers of fundamental and applied science across multiple domains, including energy and healthcare. Led by the Lab's Computational Science Initiative, researchers continue to expand analytical artificial intelligence (AI) methods, extreme-scale and streaming machine learning capabilities and "on-the-wire" processing algorithms to better process, decipher, and manage large-scale, high-volume data, including those output by major scientific user facilities, such as the National Synchrotron Light Source II.

Brookhaven Lab partners with public and private entities, providing access to unique expertise and capabilities not always readily available to industry. Brookhaven scientists are actively developing new AI/machine learning techniques and novel algorithms to control complex processes for optimizing goal-driven research. These methods aim to augment experimental design, enhance precision medicine, steer drug discovery, optimize the energy grid, and improve renewable energy production/storage. To learn more about how Brookhaven Lab's AI expertise can help your organization, visit the Brookhaven booth.

CONTACTS

Computational Science Initiative
BrookhavenLabCS@bnl.gov

Technology Commercialization
Poornima Upadhya
pupadhya@bnl.gov

Martin Schoonen
mschoonen@bnl.gov

Fermilab

Fermi National Accelerator Laboratory

Fermi National Accelerator Laboratory is America's premier laboratory for particle physics and accelerator research. Our mission is to understand the grandest questions in fundamental science from elusive particles like Higgs boson and neutrinos to the structure of the cosmos to quantum information. "Big Science" necessitates cutting-edge detectors and the most powerful algorithms to analyze massive and complex datasets. Artificial intelligence is at the core of our discovery mission.

Fermilab plays a critical role in the intersection of AI, experimentation, and scientific data. Our challenges require the capability to integrate novel and intelligent sensing devices with powerful computing infrastructure for the analysis of large datasets. We bring together the entire research community, from academia and industry, to deploy AI throughout the scientific process, and our partnerships include some of the most important AI companies in the world.

Among our family of unique AI capabilities, we highlight:

- **Real-time AI and intelligent sensing and data acquisition systems.** We are leaders in the construction and operation of large-scale and high-speed data acquisition systems. We build innovative systems that meet unique challenges from AI inference in hundreds of nanoseconds to low-power, low-noise, high-speed detectors with embedded AI to enable edge computing while operating in harsh environments (deep cryogenic to high-ionising radiation).
- **Grand science with massive datasets.** Particle physics data are different from commercial data; the equations of nature underlie our measurements. Our theoretical frameworks provide novel avenues for understanding and explaining AI. Our massive data analysis challenges require living at the forefront of AI computing technology and infrastructure.
- **Control of complex systems.** We are bringing AI to the control of particle accelerators, some of the most complex detector devices in the world, and to steering telescopes to respond intelligently and efficiently to changing conditions in the sky.

CONTACTS

Charles Thangaraj
jtobin@fnal.gov

Farah Fahim
farah@fnal.gov

Idaho National Laboratory

Idaho National Laboratory (INL) is investing in the future with artificial intelligence (AI); developing the human, physical, and virtual cyberinfrastructure needed to advance science; to grow and maintain the United States global advantage; and to ensure national security. INL researchers and trainees are investigating the development of new forms of AI, utilizing AI to support pioneering research endeavors, and conducting outcomes-based experiments harnessing the power of AI for real-world scenarios.

The new Cybercore Integration Center and the Collaborative Computing Center (C3) at INL will facilitate the alliance between industry, government, and academia critical for research and application of AI; aid in training the next generation of AI-capable researchers; and provide vital additional super-computing capacity.

Machine learning is transforming battery and catalysis research by mixing expert knowledge in energy physics with experimental kinetics data to seed development of an explainable AI, a unique collaboration between unsupervised machine learning and human input. To study the atomic environment, researchers are applying AI for analysis of extended x-ray absorption fine structure data. AI is even facilitating nuclear material imaging analysis.

Across the laboratory, projects are developing AI-powered autonomous control systems for energy production and incident response. Biofuels researchers are harnessing AI to optimize highly variable processing procedures towards the most economically viable products. INL cybersecurity researchers have developed the Autonomic Intelligent Cyber Sensor (AICS) to use AI to monitor and protect industrial control systems from cyber threats. AICS and SOPHIA, a system that monitors communication pathways for network security, are some of the numerous AI products developed by INL to shield critical United States infrastructure.

AI is revolutionizing research at INL. Fueled by advancements in machine learning, rapid and exponential expansion of data, and increasing capacity for supercomputing, INL is at the forefront of national efforts in AI research and AI-based technologies for energy and cybersecurity.

CONTACTS

Leah Guzowski
leah.guzowski@inl.gov

Ryan Bills
ryan.bills@inl.gov

BERKELEY LAB

Lawrence Berkeley National Laboratory

At Berkeley Lab, computer scientists, mathematicians, and domain scientists are collaborating to turn burgeoning datasets into scientific insights through machine learning (ML).

With five DOE national user facilities (for nanotechnology science, high-performance computing, synchrotron x-ray research, networking, and genomics), world-class applied mathematics, computer and computational science, and a pool of scientific talent that has produced 13 Nobel laureates, scientific ML has found fertile ground at Berkeley Lab.

Thanks to better instruments, we can see things at a microscopic and atomic scale. We can measure vibrations imperceptible to the human eye, and capture high-resolution images of objects millions of light-years away. But those instruments produce vastly larger datasets than ever. The Large Synoptic Survey Telescope will produce 20 terabytes of data every night, about 60 petabytes over its lifetime. The Large Hadron Collider will have even more, with 50 petabytes in 2018 alone and 500 petabytes by 2024. Conventional data analysis alone can't keep up.

With ML, models are automatically derived from data. These models can be used to identify features, reduce complexity, and control experiments. But scientists need to explain their findings, so Berkeley Lab's research into ML builds on its foundational work in mathematics to develop methods that are consistent with physical laws, robust in the presence of noisy or biased data, and capable of being interpreted and explained in scientifically meaningful ways.

Using ML in over 100 different projects, Berkeley Lab scientists have tracked atomic particles, searched for better battery materials, analyzed traffic patterns, improved crop yields, pinpointed extreme weather in exascale climate simulations, and pieced together metagenomic puzzles from billions of DNA fragments. As a Department of Energy National Laboratory, we also develop and share the algorithms, software, tools, and libraries that are foundational to scientific ML. And, we're just getting started.

CONTACTS

Todd Pray
tpray@lbl.gov

Sebastian Ainslie
sainslie@lbl.gov

Lawrence Livermore National Laboratory

Lawrence Livermore National Laboratory

Data science, encompassing artificial intelligence, big-data analytics, computer vision, machine learning (ML), predictive modeling, statistical inference, and uncertainty quantification, has thrived in Lawrence Livermore National Laboratory's (LLNL) data-focused environment. LLNL data science advancements are used institution-wide to accomplish strategic goals in a broad range of disciplines, such as predictive biology, climate research, astrophysics, advanced manufacturing and materials, simulation science, energy, and national security.

- LLNL is advancing a new class of simulations — called cognitive simulations — that uses machine learning to help scientists improve simulation models through the integration of simulated and experimental data. This new high-dimensional ML modeling capability will provide researchers with effective predictions, reliable UQ estimates, and, ultimately, new scientific understanding.
- Data science techniques are at the heart of projects focused on accelerating materials discovery, optimization, and deployment processes, creating feedstock materials that can be synthesized and optimized for system-level integration and meet performance requirements with predictive behaviors.
- Livermore and its partners are working together to apply advanced computing to biological research — integrating supercomputing, data analysis, and predictive modeling at scale and changing the way biological research is done to make the world a healthier and safer place. The ATOM (Accelerating Therapeutics for Opportunities in Medicine) and TRACK-TBI (Transforming Research and Clinical Knowledge in Traumatic Brain Injury) consortia are two successful collaborations to emerge from this area of work.

An expert, interdisciplinary workforce and extreme computing resources underlie LLNL's data science advancements. LLNL is home to Sierra, the second fastest supercomputer in the world, and the recently announced El Capitan, DOE's third exascale-class supercomputer. LLNL's Data Science Institute (DSI) acts as the central hub for all data science activity at LLNL, working to help lead, build, and strengthen the data science workforce, research, and outreach to advance the state-of-the-art of our nation's data science capabilities.

CONTACTS

Charity Follett
follett2@llnl.gov

Candace Gellner
gellner2@llnl.gov

Los Alamos National Laboratory

Los Alamos National Laboratory is changing the way we do science—and will continue to press the boundaries of the possible.

New artificial intelligence tools contribute to Los Alamos National Laboratory's national security mission,as well as everyday applications, such as strengthening our electric grid, unpacking the physics of earthquakes, understanding disease outbreaks, creating innovative new materials, and enhancing cybersecurity. In some instances, Los Alamos has applied existing AI tools to novel problems. In others, the Laboratory has developed new approaches to AI and machine learning. Los Alamos plays a key convening role in the community, hosting international workshops and summer schools to foster an exchange of ideas and find solutions to some of the world's biggest AI challenges.

Highlights of recent AI-enabled work at Los Alamos include:

- Experimenting with inserting AI algorithms into the large-scale computational physics codes that generate mission-critical hydrodynamic simulations for nuclear stockpile stewardship.
- Using an approach based on language-translation software to develop AI tools to rapidly identify patterns across malware samples that have been disguised by attackers.
- Developing tools that apply physics-based AI optimization techniques to the electric grid to detect anomalies and identify severe natural and human-made threats, thus reducing power disruptions.
- Using expertise in supercomputing and AI-tool development to accelerate cancer research, develop an AI approach to detect potential re-emergence of deadly disease outbreaks, and apply AI and machine learning to a vast HIV genetic database to design a "mosaic" vaccine.
- Creating AI algorithms and machine-learning tools to comb through mountains of statistical data to find telltale acoustic signals emitted by faults that precisely predict the time remaining before the next fault slip.

CONTACTS

Michael Everhart-Erickson
michaele@lanl.gov

Kaelyn Badura
kbadura@lanl.gov

NATIONAL ENERGY TECHNOLOGY LABORATORY

National Energy Technology Laboratory

National Energy Technology Laboratory (NETL) is pursuing artificial intelligence (AI) and machine learning (ML) approaches for fossil energy technologies. Examples include:

- Construction of the Center for Data Analytics and Machine Learning, which is accelerating the Lab's ability to process large amounts of data more efficiently.
- Providing insight into plant operations using computational fluid dynamics (CFD) and ML.
- Expanding current work to develop the next generation of methane leak detection technology using an AI aerial platform.
- Collaborating with other national labs to advance the eXtremeMAT research effort with the goal of using ML to reduce cost and time when developing novel materials for fossil energy applications like heat-resistant alloys.
- Describing the behavior of subsurface systems through complex and rapid empirical models enabled by ML.
- Using ML approaches in coordination with the Lab's Energy Data Exchange to solve challenges faced by researchers needing to effectively use data resources.
- Integrating ML techniques into the Institute for the Design of Advanced Energy Systems — a computational platform that enables innovation and large, multi-scale system optimization — to enable automated development of thermodynamic, physical property, and kinetic sub-models from experimental data.

The Lab is also amplifying its impact through NETL-managed projects with our partners across the nation. Examples using AI and ML techniques include:

- Using unsupervised ML techniques to understand operational conditions and flag anomalies in power plants (SparkCognition).
- Enabling, improving, and protecting power systems by melding traditional IT Cyber Security, Operational Technology sensor and platform information, data analytics, and ML (Southern Company Services).
- Developing autonomous robots for real-time inspection of boiler furnace walls and live repairs of cracks using AI software and smart data (Colorado School of Mines).
- Integrating real-time monitoring of power plant component conditions to enable condition-based maintenance and prediction of remaining useful life (Siemens Corporation).

NETL also leverages its recently updated supercomputer Joule, which ranks 21st in the nation (as of July 2019), for a variety of cutting-edge research and development projects such as system design and optimization for the power plants of the future.

CONTACTS

James Ferguson
james.ferguson@netl.doe.gov

Anthony Armaly
anthony.armaly@netl.doe.gov

National Renewable Energy Laboratory

While rapid advances in high-performance computing capability have traditionally expanded our knowledge and understanding, data-driven research and machine learning (ML) are emerging as the new driving force in scientific discovery toward National Renewable Energy Laboratory's (NREL) mission to transform the energy system. NREL researchers are increasingly shifting focus from understanding devices and processes — the realm of traditional modeling and simulation — to needing to develop improved designs as well as understand the interactions that occur between the devices and processes that make up large-scale energy systems.

Artificial intelligence (AI) research at NREL falls roughly into three categories: data-driven regression and classification to make sense of a deluge of simulation and measured data; data-driven model development to improve the accuracy and cost of high-throughput simulations; and generalized AI and ML to use available data to make inferences and actionable control policies.

In data-driven regression, for example, brute-force search for new materials with desirable properties can now be facilitated by a screening step that uses ML to predict the outcome of expensive simulations and experiments, thereby reducing the number of candidates to consider. For design optimization, surrogate models that balance cost against accurately relating design parameters to desired outputs are often needed — but the highest-accuracy models can easily consume a supercomputer's entire capability for days or months on end, making them invaluable for insight but infeasible to use to evaluate the multitude of necessary configurations. With the power of ML, the output of a few of these simulations can be used directly to improve high-throughput calculations that can be executed rapidly. NREL is also using reinforcement learning techniques in control strategies to experiment with the environment and update decision-making in real time to optimize operation — an exciting effort to advance the frontier of AI.

CONTACTS

Bill Farris
william.farris@nrel.gov

Erin Beaumont
erin.beaumont@nrel.gov

Oak Ridge National Laboratory

Oak Ridge National Laboratory (ORNL) applies AI to a wide variety of science and national security domains including materials science, nuclear science, satellite imagery, cyber security, urban dynamics, and health sciences. The Laboratory is particularly suited to advance AI tools for scientific research due to its unique suite of expertise, compute capabilities, and user facilities.

ORNL is home to Summit, the world's most powerful and smartest supercomputer. With hardware optimized for AI applications, Summit provides an ideal platform for applying machine learning and deep learning to groundbreaking research — the system's increased memory bandwidth allows AI algorithms to run at faster speeds and obtain more accurate results.

More than 500 ORNL researchers are using AI to accelerate breakthroughs across the scientific spectrum and develop new technologies to complement and expand these capabilities, establishing AI as a force for advancing both fundamental and applied science.

In recognition of AI's potential, ORNL has made a significant internal research investment toward an AI Initiative aimed at assisting researchers in reducing their times to solution and equipping cross-cutting research teams with novel data capabilities to tackle some of today's most complex scientific and national security challenges.

The Initiative has demonstrated new capabilities in materials science, engineering design, accelerated learning, and scalability by showing that machine learning algorithms can be used to extract information from signals with low signal-to-noise ratios; developing algorithms capable of accelerating modeling and simulation with very little training data; and designing novel biomimetic neuromorphic devices capable of detecting epileptic seizures.

Simply put, ORNL's expertise in algorithm development and its rich history of algorithm deployment in scientific applications, along with its unique data and computing infrastructure, make ORNL the ideal setting in which to realize the potential of AI in missions of national and international importance.

CONTACTS

Michael Paulus
paulusmj@ornl.gov

Suzy Tichenor
tichenorsp@ornl.gov

Pacific Northwest National Laboratory

Artificial intelligence (AI) has developed rapidly, and its presence is now felt in nearly every aspect of life. Pacific Northwest National Laboratory (PNNL) plays a significant role in advancing the fields of AI and machine learning and is applying machine learning techniques to science and engineering research to deliver solutions.

Our analytic and machine learning methods are separating useful data from noise, increasing the predictive power and efficiency of computational models, and aiding in decision-making to address important national and global issues. Contemporary machine learning research conducted by PNNL has laid foundations for a new generation of AI applications in basic science, energy, national security, and health.

Some examples of PNNL's machine learning research include the following:

- The number of sensors and Internet of Things devices is increasing rapidly as homes, businesses, and even cities, states, and nations increasingly create and track enormous amounts of spatial-related data. **Identify n-D** makes the geolocation of connected devices simple in multiple dimensions.
- Safeguarding the reliability of the electric grid requires planning for a response to the worst operating conditions. **Transformative Remedial Action Scheme Tool (TRAST)** is a powerful, automated contingency and emergency planning tool used to determine realistic remedial actions.
- The sheer number of victims when a mass casualty incident occurs can easily overwhelm first responders. **VitalTag**, a wearable wireless health monitor, sends patients' vital signs to emergency responders to aid in triage.
- Images can answer big science questions, but large image sets are challenging to organize and understand. **Sharkzor** combines user interaction with deep learning to quickly classify images by learning from a few examples.
- Active shooter incidents require rapid response from law enforcement and first responders. The **Acoustic Gunshot Detector** instantly detects a gunshot and the caliber of the fired weapon with high precision to initiate a response.

Learn about these capabilities and more at PNNL's *X*Lab booth.

CONTACTS

Kannan Krishnaswami
kannan@pnnl.gov

Scott Godwin
scott.godwin@pnnl.gov

Sandia National Laboratories

Sandia National Laboratory

Sandia National Laboratories is developing new artificial intelligence (AI) and machine learning (ML) technology to successfully fulfill our unique national security mission. To meet mission needs, Sandia must provide understanding around and quantification of uncertainty through explainable algorithms to create trusted solutions. Due to the nature of the problems we are solving, AI and ML applications frequently consist of large volumes of simulation data and very little experimental data and require instantaneous decisions. This process continues to drive innovation and produce novel techniques that address previously unsolvable problems.

Sandia performs research and development across multiple discipline areas including energy, manufacturing, transportation, risk assessment, and healthcare. Sandia leverages its AI and ML capabilities to explore novel technologies for grid stability; categorize and discriminate objects and patterns for manufacturing processes; explore neuromorphic computing applications for size-, weight-, and power-limited transportation technologies; gather and evaluate synthetic data for risk assessment applications; and employ ML for molecular dynamic applications.

Sandia pushes the boundaries in high-powered computing by exploring cutting-edge neuromorphic hardware and algorithms together in our Neural Exploration Research Lab (NERL). In addition, Sandia's Whetstone, a software tool that sharpens the output of artificial neurons, allows any AI developer to take advantage of the low-power neural-inspired computing hardware capable of processing information up to a hundred times more efficiently than the current industry standard.

These projects highlight a few ways in which Sandia is currently employing AI and ML in pursuit of our national security mission. Sandia has built these capabilities through internal projects and by collaborating with partners across the country. Come visit the Sandia booth to explore how you can leverage our state-of-the-art facilities and expertise to deliver innovative AI and ML solutions.

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

CONTACTS

Mary Monson
mamonso@sandia.gov

Joel Sikora
jsikora@sandia.gov

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Savannah River National Laboratory

At Savannah River National Laboratory (SRNL), Artificial Intelligence is utilized as a cross-cutting technology in many technical areas of interest.

NATIONAL SECURITY

- Analysis of Remote-Sensing Imagery — SRNL is automating the scanning process of commercial satellite data using algorithms to examine areas of interest to detect objects and scene change.
- A Digital Imaging and Measurement System has been developed to replace x-ray inspections that use obsolete film materials. *In-situ* digital imaging reduces variation in measurements through computerization with immediate results.
- Algorithms are being developed to identify the multi-species chemical signature "fingerprints" of processes relevant to non-proliferation. Algorithms take advantage of the higher-order dimensionality of the large data sets to convert chemical data into information for pattern recognition.
- Threat intelligence algorithms are being developed to identify anomalous traffic and extract the "Indicators of Compromise" as a means to prevent cyber-attacks and disruption of critical services.

MATERIALS SCIENCE

- AI methods, based on computer vision, are being created at SRNL to analyze imaging data for corrosion investigations and molecular modeling of corrosion processes. SRNL has developed a pre-processing graphical user interface (GUI) to improve recognition of characteristic features.

ENERGY

- SRNL is collaborating with UNC-Charlotte, Clemson University, and Duke Energy on the Grid Modernization Lab Consortium Project by developing tools for utility companies to improve response to high-impact, low-frequency events such as hurricanes.

ENVIRONMENTAL MANAGEMENT

- AI methods are being used for monitoring contaminated groundwater. Staff at SRNL and LBNL are creating a cost-effective approach for long-term monitoring based on measuring master variables, which control plume mobility and its spatial and temporal distribution and can be measured *in situ* continuously using distributed automated sensors.
- SRNL is developing an alternative imaging capability for measuring radioactive materials *in situ* using a robotic-mounted gamma-ray detector that can move around an area of interest, sampling the space at a high-frequency mapping material distribution.
- SRNL is monitoring liquid-liquid behavior in centrifugal contactors using noninvasive imaging tools coupled with CFD modeling to enhance understanding of the influence of design attributes and operating parameters on phase separation efficiency.
- Online monitoring tools and data analytics are accelerating SRS H-Canyon processing rates, reducing cost, and enhancing process understanding.

CONTACTS

Matt Biasiny
matthew.biasiny@srnl.doe.gov

Ralph James
ralph.james@srnl.doe.gov

SLAC NATIONAL ACCELERATOR LABORATORY

SLAC National Laboratory

As one of 17 Department of Energy National Labs, SLAC pushes the frontiers of human knowledge and drives discoveries that benefit humankind. We invent the tools that make those discoveries possible and share them with scientists all over the world.

SLAC IN ARTIFICIAL INTELLIGENCE (AI) AND MACHINE LEARNING (ML) FOR ENERGY, MANUFACTURING, HEALTH CARE, AND TRANSPORT:

- SLAC National Accelerator Laboratory is working with Berkeley Lab to use AI to prevent or minimize electric grid failures and bounce back faster from storms, solar eclipses, cyberattacks, and other disruptions.
- SLAC researchers are using AI and accelerated experiments to speed the discovery of new materials, such as metallic glasses and new photocathodes, in a fraction of the time and cost required for conventional discoveries. SLAC is also applying ML to materials science computational tools as part of the MAGICS collaboration.
- SLAC researchers are developing tools that will help reduce peak load impacts from uncontrolled charging, reduce local distribution system impacts from clustering of EVs, and enable us to develop methods to quantify value streams for EVs as a grid resource for both the retail and wholesale markets.
- SLAC National Accelerator Laboratory is exploring the deployment EdgeAI within detector and DAQ systems to accelerate data processing and compress large data volumes for efficient analysis. This includes inline data compression, detector triggering, and fast online analysis.
- SLAC is developing ML methods to control and monitor large, complex facilities, including through online optimization and fault detection and recovery.

Beyond the topics of the *X*Lab, SLAC has a broad range of programs applying AI and ML at our large-scale scientific facilities to drive discovery in both the fundamental and applied sciences.

Stanford University operates SLAC for the DOE Office of Science. We run four joint research centers with Stanford that focus on cosmology and astrophysics, materials and energy science, catalysis, and ultrafast science. SLAC's location in Silicon Valley and our connections with DOE, Stanford, and other leading research centers speed our progress. We also look for ways to work with industry to solve problems and spread the benefits of research out into society.

CONTACTS

Laura Schelhas
schelhas@slac.standford.edu

Ryan Herbst
rherbst@slac.stanford.edu

Thomas Jefferson National Accelerator Facility

Thomas Jefferson National Accelerator Facility (Jefferson Lab) is a single-purpose, Department of Energy national lab which serves the nuclear physics community.

Within the last year, significant progress has been made applying Artificial Intelligence (AI) to a variety of tasks. Generally speaking, the sources of data at the laboratory originate from the experimental end stations (of which there are four) or from the particle accelerator itself.

On the accelerator side, excellent progress has been made using machine learning to classify the type of accelerating cavity faults and is nearing deployment. The near real-time feedback the system will provide to control room operators is expected to increase beam availability to users. Additional work is being pursued in extracting latent knowledge from the accelerator's large, archived dataset.

On the nuclear physics side, there are multiple efforts underway which include leveraging AI for particle identification and charged particle tracking. Here there is a potential for significant savings in expensive computational time compared to conventional methods. Another system near deployment is an AI-driven data quality monitoring system to provide near real-time feedback to operators regarding the health of the detectors and the quality of data they are producing. While conventional control systems are well-suited to alert for big problems, these systems do not often catch more subtle or nuanced issues that can affect the quality of physics data produced.

Jefferson Lab is currently designing an electron-ion collider to serve as the next generation accelerator to meet the demands of the nuclear physics user community. AI is being used to guide the detector design, to extract unknown correlations from physics datasets, and to aid in efficient data reduction. The lab is actively fostering the growth and development of the emerging AI community through a weekly, labwide lunch series and other outreach opportunities.

CONTACTS

Christopher Tennant
tennant@jlab.org

Yves Robin
robin@jlab.org

U.S. DEPARTMENT OF ENERGY | Office of TECHNOLOGY TRANSITIONS

DOE Office of Technology Transitions and Laboratory Partnering Services

The U.S. Department of Energy (DOE) is one of the largest supporters of technology transfer in the federal government. The Office of Technology Transitions (OTT) was established in 2015 to develop the Department's policy and vision for expanding the commercial impact of its research investments. OTT streamlines access to information and to DOE's National Labs and facilities — fostering partnerships that guide innovations from the labs into the marketplace. The OTT Director and Chief Commercialization Officer serves as the principal advisor to the Secretary on all technology transfer and commercialization matters.

Come visit us at the OTT booth to learn more about the Department's commercialization mission, meet with our staff, and catch a demo of the Lab Partnering Service (LPS) — a powerful tool to match entrepreneurs and investors with the very best technologies (including AI!) and experts the National Labs have to offer.

CONTACTS

Peebles Squire
peebles.squire@hq.doe.gov

Robert Bectel
robert.bectel@ee.doe.gov

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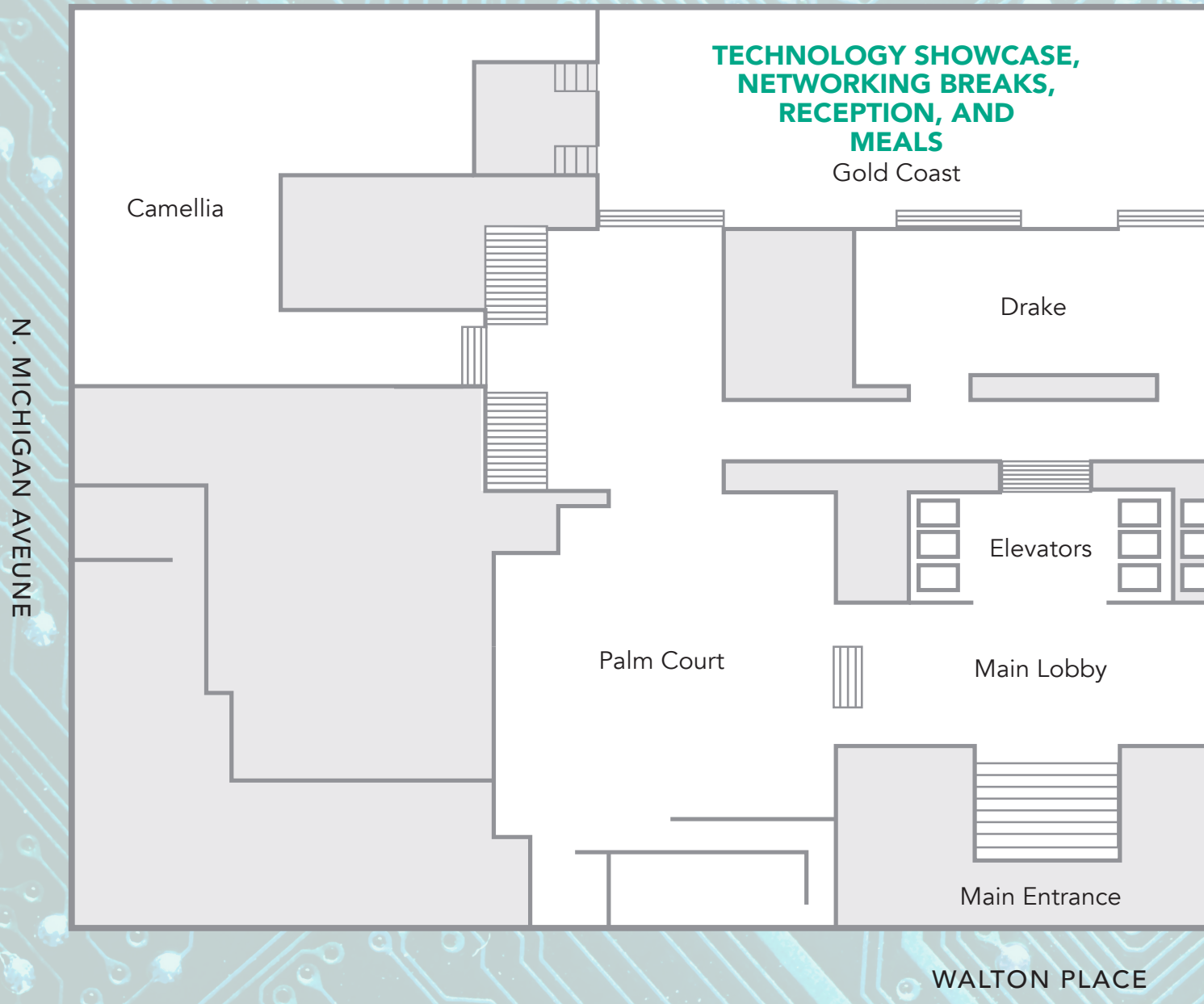
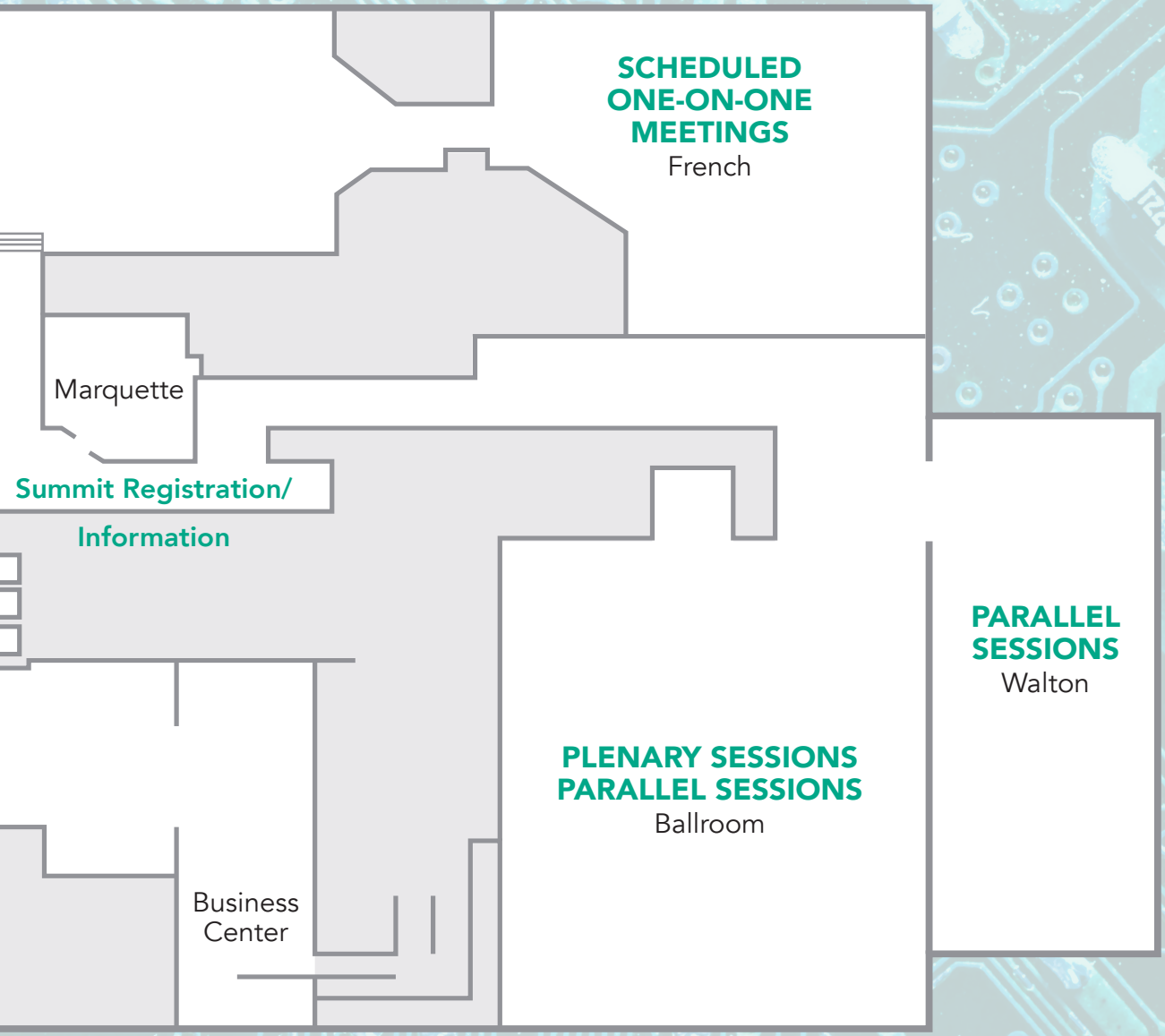
Getting Around

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