Artificial Intelligence at LLNL

Exploring fundamental AI research to advance mission-critical applications.

Accelerating Science

From Wall Street to the White House, artificial intelligence (AI) is more than a buzzword. It is a rapidly growing—yet little understood—field that has changed the world in numerous ways. At Lawrence Livermore National Laboratory (LLNL), we dig deep into all aspects of AI, investigating its capabilities alongside vulnerabilities. We develop sophisticated AI technologies while leading the conversation about using AI to advance science and address national security needs.

Amid headlines about AI startups, products, and ethics, challenges remain regarding AI safety and security—with effective solutions yet to emerge from commercial companies. As a national laboratory with a high-stakes mission to steward critical technology, we are concerned with these issues, so fundamental research is a cornerstone of our AI exploration. Additionally, our experimental facilities, high-performance computing systems, and large multimodal datasets provide a robust proving ground for developing and testing new techniques.

Driven by national security and our service-oriented role, LLNL has demonstrated leadership in using AI to tackle scientific challenges, while also creating an important link between academia and industry. This also positions LLNL to help the Department of Energy and the National Nuclear Security Administration contribute to AI-related national security solutions..

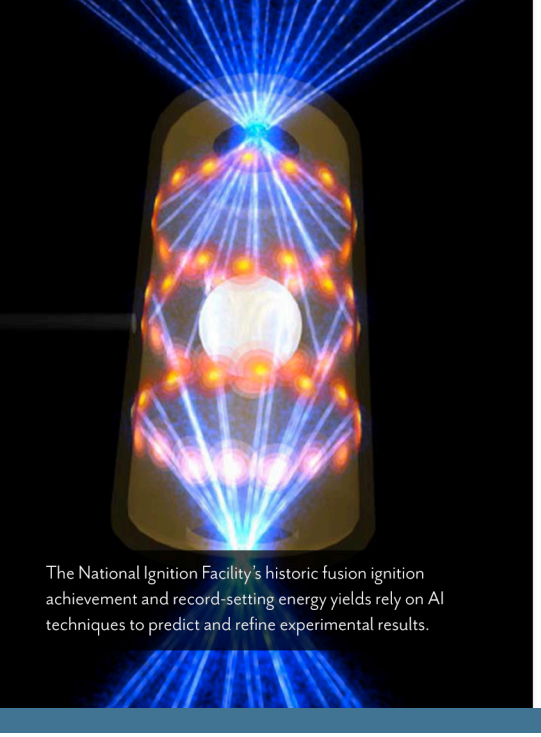
Transformational Research

AI has great potential to transform national security science in mission-critical applications, such as those related to the strategic deterrent, intelligence gathering, and nuclear nonproliferation. It allows us to combine copious simulation predictions and detailed experiments to form an incredible model of our physical world. But can the model be trusted when conditions in the lab or the field differ from the training data? Can the model make reliable predictions about key situations it has not previously encountered? LLNL is pioneering new AI technologies that meet the high standards necessary for our national security missions.

To effectively harness the power of—and increase confidence in—this transformative technology, LLNL's foundational AI research encompasses a full spectrum of safety and security considerations:

- **AI for mission-critical science:** Commercial AI solutions are impressive in their domain but not yet capable of addressing foundational challenges of national security science. We build specialized AI solutions for our critical science missions, pushing AI to handle any scientific data modality.
- **Robustness and safety:** Mainstream AI solutions are often brittle and produce nonsensical results for even minor variations on the inputs. We created small models with better adversarial robustness than larger models can achieve.
- **Generalization and uncertainty:** Many AI techniques are unable to generalize to unknown situations yet are overly confident of their predictions. Our novel frameworks and algorithms generate reliable uncertainties for high-confidence decision making.
- **Interpretability and trust:** Understanding how an AI model makes decisions is crucial to extracting scientific insights, instilling trust in subsequent decisions, and guarding against unintended biases. We explore "black box" models by visualizing high-dimensional design spaces.

The most effective AI models are resilient to outlying or anomalous data, reliable with trusted datasets, and robust against noise. LLNL is developing AI tools to address these problems, which leading companies have not been able to solve, and with results that outperform state-of-the-art models.



The National Ignition Facility's historic fusion ignition achievement and record-setting energy yields rely on AI techniques to predict and refine experimental results.

From custom feedstocks to digital twins, AI-enabled materials development and advanced manufacturing processes often lead to industry collaborations.

AI in Action

LLNL's leadership in AI requires robust community engagement, both inside and outside the Lab. Through our AI Innovation Incubator, we form public/private partnerships and share our interdisciplinary scientific challenges with industry leaders. Our Data Science Institute supports our workforce through educational and collaborative opportunities. Additionally, we mentor the next generation of AI experts through student internship programs. These activities along with strategic, multi-year investments in AI research are already making a difference as we integrate AI into a wide variety of applications:

- **Inertial confinement fusion:** We combine AI surrogate models with simulations and data to predict fusion experiment performance and improve laser shot designs. The National Ignition Facility's diagnostic tools generate datasets for every shot, which are fed into AI models to inform future shots.
- **Advanced manufacturing:** We augment manufacturing processes with generative AI techniques enable adaptive design and smarter production operations. We are working with industry partners to build laboratories that autonomously manufacture parts and optimize designs.
- **Drug design:** We co-founded a consortium that develops AI tools to accelerate the drug discovery pipeline. These tools characterize billions of compounds, so only the most promising molecular combinations—those targeting cancer cells or viruses like COVID-19—move on to the costly experimental phase.
- **Cancer modeling:** RAS proteins are a family of proteins whose mutations are linked to more than 30% of human cancers. We developed an AI-based simulation framework that models RAS protein biology at different spatial and temporal scales: from nano- to milliseconds and from nano- to micrometers.
- **Strategic deterrent:** We built AI models to assess the reliability of the nation's nuclear stockpile. These models accelerate precision simulations, tune experimental facilities (e.g., Scorpius accelerator), guide optimized system designs, and distill information from empirical observations.
- **Image reconstruction:** Computed tomography (CT) reveals an object's interior by piecing together x-ray images. We developed AI tools to 3D-reconstruct an object for better anomaly detection in settings where only limited CT views are available, such as hospitals and airport security screening.
- **Materials synthesis:** We created AI techniques to expedite the discovery, optimization, and deployment of different types of materials, such as high explosives. These projects include using machine learning and computer vision to predict which physical features are important.
- **Model safety and trust:** We developed neural network compression approaches that show for the first time that AI robustness and efficiency are not mutually exclusive. These smaller AI models outperform significantly larger models from industry leaders.

The Future

The only certainty in AI is that opportunities and challenges abound. At LLNL, we recognize the need to balance innovation and preparedness in this burgeoning field, especially regarding the nation's security and stability. Whether improving cybersecurity infrastructures, boosting the accuracy of clinical predictions, or developing tools that explain how AI models work, our researchers evaluate and leverage new AI paradigms and technologies (e.g., the advent of large language models) in the context of our mission. Additionally, we are planning activities to collaborate with other national labs, including increased data sharing. Under LLNL's Cognitive Simulation Institutional Initiative, we will uphold a deliberate, focused vision for AI development and execution in addressing national security priorities.

Learn More

LLNL's AI research includes these frequently cited papers:

- Diffenderfer J., et al. "Multi-Prize Lottery Ticket Hypothesis: Finding Accurate Binary Neural Networks by Pruning a Randomly Weighted Network." International Conference on Learning Representations (ICLR), 2021.
- Xu K., et al. "Automatic Perturbation Analysis for Scalable Certified Robustness and Beyond." Neural Information Processing Systems (NeurIPS) Conference, 2020.
- Thiagarajan J.J., et al. "Single Model Uncertainty Estimation via Stochastic Data Centering." Conference on Neural Information Processing Systems (NeurIPS), 2022.

Learn more about our research in high-impact publications along with our AI-related patents, open-source datasets, and open-source software:

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