Los Alamos National Laboratory
Energy Infrastructures Portfolio
Strategic Capability Survey

Los Alamos
NATIONAL LABORATORY

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Contents

1 Introduction

Following the U.S. test-ban treaty for nuclear weapons, Los Alamos National Laboratory (Los Alamos or Laboratory) developed an advanced modeling and simulation capability to ensure the reliability of the U.S. nuclear arsenal. This legacy has evolved into cutting-edge capabilities in modeling, simulation, and applied mathematics to inform scientific experimentation in many research areas, including energy systems.

In energy systems research, the National Infrastructure Simulation and Analysis Center (NISAC), a program created by the U.S. Department of Homeland Security, utilizes Los Alamos' modeling and simulation tools to identify the vulnerabilities and failure modes of a broad selection of critical national infrastructures. NISAC provides comprehensive, quantitative analyses to better understand the wide variety of threats and solutions to the nation's infrastructures. Through internal Laboratory Directed Research and Development (LDRD) investments and subsequent partnerships with the U.S. Department of Energy's (DOE) Office of Electricity (OE), Los Alamos has built on this expertise to support the modernization of the Nation's electrical grid and critical energy infrastructures, utilizing three guiding principles:

1. focusing fundamental research on areas of need within the Los Alamos national security mission;
2. fostering interdisciplinary thinking through education, workforce development, and collaboration; and
3. prioritizing transition of scientific results, analysis and capabilities to the broader community.

To support OE programs, Los Alamos leverages its capabilities in physics, network science, algorithms, and applied mathematics to develop fundamentally new algorithms and methods for designing, controlling, and optimizing future energy systems, such as electrical grids. For example, Los Alamos has developed advanced control approaches and optimized system response to support the integration of intermittent resources, such as renewables, and mitigate the effects of uncertain energy production these resources pose. Los Alamos has also supported OE initiatives to develop approaches to design resilient energy systems that combine hardening the existing system and the introduction of redundancy.

This document reviews Los Alamos' research and development (R&D) capabilities in planning, modeling, analyzing, and optimizing interdependent and interconnected energy infrastructures. It provides remarks on how these capabilities may be used to support the DOE in achieving its priorities of:

- *Decarbonization* — reducing carbon dioxide and other greenhouse gas emissions from our atmosphere;
- *Infrastructure Modernization* — investing in energy infrastructure improvements and commercialization of technologies currently in the R&D phase;
- *Equity and Energy Justice* — partnering with historically disadvantaged communities to ensure a just and equitable energy transition and making sure that those who have suffered the most are the first to benefit from the clean energy revolution; and
- *Climate Adaptation and Mitigation* — reducing emissions and stabilizing the levels of heat-trapping greenhouse gases in the atmosphere ("mitigation"), and adapting to the climate change already in the pipeline ("adaptation").

Introduction

To enable a just transition to a carbon-neutral energy sector by 2035 and a net-zero emission economy by 2050 – while maintaining the reliability, affordability, security, and resilience of the energy system – DOE is partnering with national laboratories, universities, and industry partners to advance these goals.

DOCUMENT ORGANIZATION

In this document, Los Alamos' overall ***Laboratory Vision*** is introduced in **Section 2**, highlighting the mission and values of our organization that informs our approach to supporting the DOE OE.

Los Alamos' approach to R&D in energy systems planning and modeling, and in analyzing and optimizing energy infrastructures, are organized around two intertwined themes: ***Core Capability Development***, discussed in **Section 3**; and ***Supporting DOE Priorities***, discussed in **Section 4**. Our philosophy for developing core capabilities follows the pyramid framework presented in Figure 1-1 and is introduced below. The second theme is structured around the DOE's priorities and suggests pathways for how Los Alamos' capabilities may be used to support these goals.

In Figure 1-1, the foundation of Los Alamos' research and support of the DOE are the *Fundamentals*, the basic science of Los Alamos' capabilities. These, upon *Implementation*, create core building blocks, which enable the construction of capability *Tools* for solving specific problems (i.e., take input(s) and produce output(s)). At the top is the *Analysis*, the strategic, cutting-edge capabilities that are used to support a variety of critical objectives and national missions. Each layer builds upon the one below, combining individual components into sophisticated capabilities. *This approach ensures that capabilities can be re-purposed to meet evolving priorities of the DOE, and separates methods from specific data for transferable approaches.*

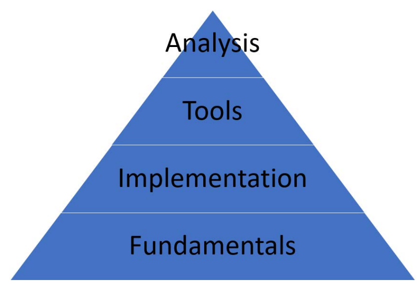


Figure 1-1: Pyramid framework structure of Los Alamos' energy system modeling capabilities.

With this organizational structure, Section 3 and Section 4 may be read in two ways: The first way is a traditional sequential read, where Section 3 describes where Los Alamos is today, before moving onto Section 4 with a discussion on how Los Alamos can support the DOE, and specifically OE, in achieving its goals. The second way is to start with Section 4, where the document considers the types of analyses Los Alamos can support, and then refer back to prior material for more detailed explanations and references on how those analyses are accomplished.

The review of Los Alamos' R&D philosophy is followed by summaries of featured ***Selected DOE Projects*** in **Section 5**, which highlight how OE programs leverage Los Alamos' capabilities and how Los Alamos furthers overarching goals of the DOE.

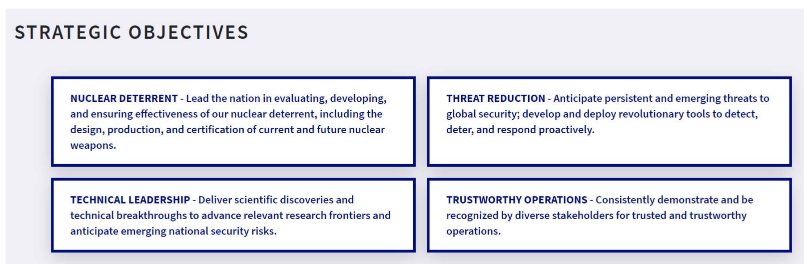
Finally, Los Alamos' ***Partnerships and Pipeline Office*** is introduced in **Section 6**, a key organization that makes Los Alamos science, technology, and engineering collaboration and recruitment possible by providing the structure and resources needed for these efforts.

2 Laboratory Vision

"SIMULTANEOUS EXCELLENCE"

As a federally funded R&D center, Los Alamos National Laboratory aligns its strategic plan with priorities set by the DOE's National Nuclear Security Administration (NNSA) and key national strategy guidance documents. The Laboratory executes work across all DOE's missions: national security, science, energy, and environmental management. Capabilities developed through Los Alamos stockpile research are leveraged to meet the Laboratory's diverse national security missions.

Mission-focused science, technology, and engineering is a key component of the Laboratory's top-line strategy of "*Simultaneous Excellence*" in nuclear deterrence; science, technology, and engineering (STE); operations; and community. To make the strategy actionable, a **Lab Agenda** is published every year, which provides a structured framework that identifies the objectives, critical outcomes, near-term R&D, and production and mission-support activities needed to accomplish our mission.



Climate and Clean Energy is one of 13 Critical Outcomes outlined in the 2023 Lab Agenda. It focuses on enabling regional and national achievement of Administration 2030/2050 climate and clean energy objectives through scientific, technological, and partnership innovations that build on established Los Alamos capabilities. **Initiatives** that fall under this Critical Outcome aim to achieve one or more of the following:

1. Enhance the capability to forecast at regional scale impacts of the evolving climate to enable science-based civilian and military actions both domestically and globally, particularly at the sub-decadal scale and integrated with weather, infrastructure, disease, and other models. Deploy Los Alamos tools to decision makers.
2. Demonstrate leadership, with relevant partners, in the multidisciplinary experimental R&D needed to inform near- and long-term predictions that influences action, as well as provide technical options to support those actions.
3. Develop, with relevant partners, utilizing a place-based strategy, innovative technology that can mitigate climate change, address the impacts of climate change, and enable monitoring of international norms and agreements.

4. Inform and facilitate implementation of a rapid transformation of the energy system towards less carbon-intensive solutions domestically, which will be paralleled by a transformation of the global energy system.
5. Support NNSA in establishing and achieving climate mitigation goals, including using the Laboratory as a testbed for demonstration and deployment efforts.

To achieve this Critical Outcome, Los Alamos builds on its existing applied energy, civilian nuclear energy, and basic energy sciences portfolios. The Applied Energy Program Office serves as the Laboratory's primary interface with most of the DOE energy programs, including OE. Los Alamos has a long history of leveraging its core science and technology capabilities to support the nation's energy security mission—a symbiotic relationship that enables an agile Laboratory response to the nation's most pressing energy challenges.

The **2023 Lab Agenda** demonstrates a strong commitment to the Administration's 2030/2050 climate and clean energy objectives, including several initiatives that align with OE goals and objectives.

As an example, Los Alamos leads the Intermountain West Energy and Sustainability Transitions (**I-WEST**) initiative, which is focused on developing a regional energy transition roadmap for six Intermountain Wests that encompass numerous communities heavily dependent on fossil-based economies. Leveraging expertise, tools, and other capabilities at Los Alamos that were developed by OE, I-WEST has made key findings related to the regional energy sector, including its impact on carbon emissions, regionally relevant pathways for decarbonization, and impacts on the regional workforce. Place-based concerns and challenges have also been identified, such as 1) balancing the production variability of renewables, 2) grid oversubscription in certain regions and the possible need for increased transmission capacity, and 3) general siting issues involving land ownership. I-WEST is now exploring how the National American Energy Resilience Model (**NAERM**) can be leveraged to conduct more in-depth analyses that can help address some of these issues and provide energy communities with region-specific data to support energy transition planning.

As part of its Climate and Clean Energy initiatives, Los Alamos partners with industry, colleges and universities, communities, and other national laboratories to deliver critical outcomes that help propel the national toward a clean energy future, while considering diversity, equity, and inclusion (DEI) as well as energy, environmental, and social justice (EESJ). The Lab Agenda's **Force For Good** critical outcome aligns with the DOE's priorities for DEI and EESJ with several initiatives focused on leveraging Laboratory technologies, expertise, and networks to build a sustainable, secure, and equitable future.

Lab Agenda Snapshot

2023 Update

The Laboratory Agenda provides a structured framework that identifies the strategic objectives, critical outcomes, near-term R&D, and production and mission-support activities needed to accomplish our mission.

Strategic Objectives

Nuclear Deterrent
Lead the nation in evaluating, developing, and ensuring effectiveness of our nuclear deterrent, including the design, production, and certification of current and future nuclear weapons.

Threat Reduction
Anticipate persistent and emerging threats to global security; develop and deploy revolutionary tools to detect, deter, and respond proactively.

Technical Leadership
Deliver scientific discoveries and technical breakthroughs to advance relevant research frontiers and anticipate emerging national security risks.

Trustworthy Operations
Consistently demonstrate and be recognized by diverse stakeholders for trusted and trustworthy operations.

Critical Outcomes

Pit Production
Reconstitute optimized rate production of pits leveraging the nation's Plutonium Center of Excellence (Pu CoE) to support deterrence.

Non-Nuclear Production
Develop targeted non-nuclear production capabilities to address gaps in the national Nuclear Security Enterprise (NSE).

Computational Breakthroughs
Research, develop, and routinely apply world-leading computational methods, approaches, applications, and technologies to solve Los Alamos' most computationally challenging science and security problems.

Experimental Advances
Advance LANL's experimental characterization tools in conjunction with our computational advances to underwrite stockpile assessment without the need for a nuclear test.

Integrated Deterrence
Develop, and demonstrate capabilities to strengthen U.S. deterrence across the competition-conflict spectrum.

Technology Modernization
Optimize and apply advanced technologies to enable modernization of the deterrent and its nuclear warheads.

Quantum Leadership
Assert LANL leadership in the National Quantum Initiative; enable emergent scientific and national security needs by advancing quantum-relevant capabilities in materials, algorithms, simulation, and devices.

Threat Response
Develop and deploy technical solutions supporting future nonproliferation, counterproliferation, and counter-terrorism strategies.

Biosecurity Preparedness
Enable national preparedness and response to infectious diseases and biosecurity threats by harnessing life sciences along with other innovative scientific approaches.

Climate & Clean Energy
Enable regional and national achievement of Administration 2030/2050 climate and clean energy objectives through scientific, technological, and partnership innovations that build on established LANL capabilities.

Operational Capacity
Meet the capacity requirements necessary to perform current and future mission.

Culture Enhancements
Champion enhancements to our work environment that support inclusive staff engagement, respectful behaviors, and learning opportunities that are the foundation for safe, secure, compliant, and quality performance of our missions.

Force for Good
Be recognized as a force for good by Northern New Mexico communities and trusted by stakeholders to perform missions with minimal operational issues.

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3 Core Capability Development

3.1 Fundamentals

Fundamentals, the basic science of energy systems research, stem from Los Alamos' national security expertise in physics, network science, and applied mathematics. These fundamentals, in areas like advanced computational algorithms and artificial intelligence, have been strategically developed and advanced over the past decades by the Laboratory. Investments in fundamentals produce prototypes at low Technology Readiness Level (TRL) and form the basis for the higher TRL products discussed later in this section.

Advanced Computational Algorithms are innovative solutions for large-scale, complex problems. These cutting-edge capabilities enable advanced modeling and simulations of energy systems – to design, control, and optimize both present-day and future critical energy infrastructures.

In the area of advanced algorithms, Los Alamos has developed a significant number of foundational applied mathematics applicable to energy systems. One of the Laboratory's primary contributions are novel ways of formulating problems to handle different representations of the physics of energy infrastructures. These include different methods for approximating (e.g., the direct-current (DC) model of power systems) or relaxing the physics (e.g, linear models, convex models, etc.) to improve computational performance of energy systems modeling and methods for handling both steady-state and transient phenomenology in energy systems. These formulations have yielded new algorithms for solving problems of interest – both deterministic and probabilistic – like the N-k interdiction problems, economic dispatch problems, optimal response to fluctuations in renewable energy production, and infrastructure restoration and resilient reconfiguration problems [1]–[5].

These foundational computational algorithms are available in open-source software libraries through capability *Implementation*s. ***Appendix A*** contains information about specific software libraries developed by Los Alamos, such as optimization solvers.

Artificial Intelligence Techniques are the basis for capabilities like robust and reliable learning and data analytics methods for use in energy systems. Much of the R&D in artificial intelligence (AI) and machine learning (ML) have focused on developing off-the-shelf, black-box technologies with greatly limited capabilities to ensure robustness, provide interpretable results, or support explainability. Related research has limited usefulness in high-consequence national security environments, such as energy systems, therefore, Los Alamos has focused on developing and implementing cutting-edge ML that address these gaps so AI can be trusted and used in such contexts.

These techniques include: physics-informed algorithms to identify anomalies and intrusions in infrastructure systems in real-time, such as Multi-Variate Anomaly Detection[1]; statistical-learning based methods to determine the reliability valuation of existing sensing technologies and support the deployment of new advanced measurement technologies to enhance infrastructure reliability; and learning assisted optimization techniques for efficient and reliable uncertainty management and decision making [6]–[11].

[1] `https://github.com/lanl-ansi/MVAD`

3.2 Implementation

Implementation is the software realization for transforming *Fundamentals* into capability building-blocks for modular reuse. These capabilities – such as simple codes and software libraries – enable the construction of more complex *Tools*. Implementations are grouped into *InfrastructureModels*, a set of software libraries for handling data and the different ways of modeling infrastructure networks, and implementations of *Problem Specifications*.

InfrastructureModels[2] is an integrated, open-source software ecosystem for co-modeling infrastructure networks from an optimization perspective. *This ecosystem provides a complimentary co-optimization capability to the DOE's co-simulation capabilities like HELICS.* Each software package in the ecosystem supports continuous integration and validation with industry standard software (e.g., PSSE, OpenDSS, EPANET, etc.) and undergoes rigorous external peer-review for correctness, exemplary software quality, and usability [12]. Each package supports industry-relevant datasets with established data formats and follows best practices for modern software design. The flexible and extensible design enables multi-infrastructure modeling and adding new infrastructure sectors with minimal time-and-effort [13].

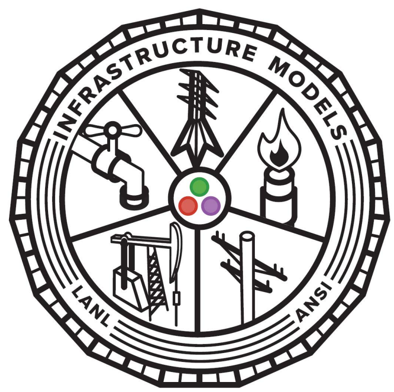

Figure 3-1: InfrastructureModels software ecosystem brand.

InfrastructureModels currently supports optimization modeling of five key infrastructure sectors: electrical power transmission (**PowerModels**), natural gas transmission (**GasModels**), petroleum product transmission (**PetroleumModels**), electrical power distribution (**PowerModelsDistribution**), and potable water distribution (**WaterModels**) systems. Less mature implementations include CO_2 pipeline transport (**CarbonModels**) and plans to develop implementations for communication and hydrogen in the future. Additionally, packages have been developed for multi-infrastructure modeling and optimization – between electrical power transmission and distribution (**PowerModelsITD**), natural gas transmission and electrical power transmission (**GasPowerModels**), and electrical power distribution and water distribution (**PowerWaterModels**) – to help improve understanding of the interdependencies between these infrastructures. ***Appendix B*** contains additional information about each of these packages.

Problem Specifications are implementations of a collection of foundational problems that arise in the design and operations of energy systems. These large-scale, complex computational and optimization problems form the validated basis for analytical tools. Each problem specification is constructed from packages in the **InfrastructureModels** software ecosystem.

[2] `https://github.com/lanl-ansi/InfrastructureModels.jl`

Implemented *Problem Specifications* include:

Flow problems – such as power flow, gas flow, water flow, gas-power flow, and power-water flow – for modeling and validating feasible flows and network parameters for an infrastructure system.

Optimal Flow problems – such as optimal power flow, optimal gas flow, optimal petro flow, optimal water flow, and optimal power-water flow – for applications that require models that minimize the costs of infrastructure system operation.

Network Design problems – such as expansion planning of electrical power transmission and natural gas transmission networks – for applications that require models that optimize infrastructure system design (e.g., minimize the cost of updating or modifying a system).

Minimum Load Shedding and *Maximum Load Delivery* problems – for electrical power and natural gas networks – for applications that optimize infrastructure system operation to model reliability and resilience.

Optimal Transmission Switching problem – for electrical power transmission networks – for analyses that models changes to infrastructure system topology to improve operation and protect equipment from damage.

These specifications are core (often academic) building-blocks for the more complex *Tools* and *Analysis* discussed later in this review and rely on the foundational modeling and algorithms discussed in the previous subsection.

3.3 Tools

Software *Tools*, are constructed from the capability building-blocks of *Implementation*(s), and are designed to solve specific problems of interest to the DOE and other federal sponsors. These capabilities, such as purpose-built software, enable decision-makers to carry out a variety of complex *Analysis* work-flows for national security. A short description of some of these tools are described below.

PowerModelsProtection[3] is a tool that uses the PowerModels and PowerModelsDistribution software libraries to model protection coordination of electrical power transmission and distribution networks. It is primarily used for modeling and assessing the reliability of protection for micro-grids and distribution networks with distributed energy resources, including both synchronous and inverter-interfaced generation, to conduct fault study and short-circuit analysis. The modeling approaches have been peer reviewed in [14], [15]. *It must be noted that this tool is less mature than other similar software tools and is under active development.*

[3] `https://github.com/lanl-ansi/PowerModelsProtection.jl`

Core Capability Development

PowerModelsRestoration[4] is a software tool that uses the PowerModels software library to model and optimize power system restoration after large-scale disruptions. The core building-block for the restoration modeling tool is the maximum load delivery problem, discussed in *Implementation*s, for calculating the size of a power outage; this provides a reliable numerical method for solving challenging N-k damage scenarios that require restoration, such as scenarios that arise in the analysis of extreme weather events. The tool has been peer reviewed in [16], [17].

PowerModelsGMD[5] is a tool built from the PowerModels and PowerModelsRestoration software libraries for evaluating the risks and mitigating the impacts of geomagnetic disturbances (GMDs) and E3 high-altitude electromagnetic pulse (HEMP) events on electrical power transmission networks. It solves for quasi-dc line flow and ac power flow problems in a system subjected to geomagnetically induced currents (GIC) and calculates GICs based on analyst provided geoelectric fields. The tool has been peer reviewed in [18], [19].

PowerModelsONM[6] is a tool built from the PowerModelsDistribution, PowerModelsProtection, and PowerModelsStability software libraries for modeling operation and restoration of electric power distribution feeders featuring networked microgrids. It focuses on optimizing the operations and restoration of phase unbalanced (multiconductor) distribution feeders that feature multiple grid-forming generation assets (e.g., solar PV, diesel generators, energy storage) and planning how to network microgrid together to improve system resilience.

SimCSS[7] is an economic-engineering software tool for decision support and design of integrated carbon capture, utilization and storage technologies (CCUS). SimCCS supports decision making by integrating applications in operations research, geographical information systems, carbon capture engineering, pipeline infrastructure design and geologic reservoir performance. Users can produce integrated CCUS system designs for problems ranging from single facilities to large, regional networks involving multiple carbon emission sources and geologic sinks. It can create candidate transportation routes and formalizes an optimization problem that determines the most cost-effective CCUS system design. By harnessing the power of high-performance computing resources, users can investigate how CCUS may play a meaningful, cost-competitive role in mitigating carbon emissions [20].

These *Tools* rely on the *Implementation*s as building-blocks to solve specific problems that are used to produce *Analysis* discussed next.

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[4] `https://github.com/lanl-ansi/PowerModelsRestoration.jl`
[5] `https://github.com/lanl-ansi/PowerModelsGMD.jl`
[6] `https://github.com/lanl-ansi/PowerModelsONM.jl`
[7] `https://simccs.org/`

3.4 Analysis

Analysis is the collection of strategic, cutting-edge capabilities of Los Alamos, which rely on *Tools* to support a variety of critical objectives and missions. These are the highest TRL products and are used to advance Los Alamos' national security mission as applied to the DOE's goals of decarbonization, infrastructure resilience, social equity, and economics. Below examples of analysis performed using *Tools* and *Implementations* are outlined. Specific government and industry users of these analytical tools are called out in specific project highlights later in **Section 5**.

Infrastructure Investment is an optimization and physics-based analysis for identifying and recommending infrastructure investments that best meet user specified criteria (e.g., resilience, capital costs, operating costs, CO_2 reduction, etc.). The analysis capability has been used to improve the resilience of critical infrastructure systems, identify and introduce hardening redundancy into infrastructures, support planning for a carbon-neutral energy future, and provide guidance on how the interconnected energy infrastructures of the U.S. should evolve to meet energy demands and clean energy targets [21]–[23].

Infrastructure Reliability Assessment is a physics-and-optimization-based, predictive analysis for understanding the behavior of independent or interconnected energy infrastructure systems. It is used for a "what if" analysis where a user posits different scenarios to understand how the system(s) reacts to those circumstances and what the best possible outcome could be.

Infrastructure Performance Planning is an optimization and physics-based modeling analysis for identifying the best plan and policies for operating independent or interconnected energy systems to meet user specified criteria (e.g., economics, mitigation to disruptions, etc.). The approach is used to calculate optimal operation conditions for various infrastructures, optimize resilience for distribution and transmission networks, and recommend optimized responses to threats [24], [25].

Pipeline Re-purposing Planning is an optimization and physics-based modeling analysis under development that is used to ensure a seamless transition to a clean hydrogen (H_2) economy in the coming decades. To achieve this goal, existing natural gas pipeline infrastructures can be utilized and upgraded to perform more compression and increase capacity for H_2 transport. Blending H_2 with natural gas would enable existing natural gas pipelines to carry varying amounts of H_2, an easy first step to developing a market for H_2 as an energy source in the near future and also as a viable approach to gradually transition to pure H_2 transport later. This would allow the Nation to leverage its existing pipeline network resource, avoid stranding assets, and preserve some of the jobs associated with operating fossil-based systems. **GasModels**, **GasPowerModels**, and other tools of the **InfrastructureModels** software ecosystem directly support planning, decision making, and implementation activities. Achieving the aforementioned goal, however, requires the development of physical models for blended gases to avoid erroneous conclusions.

Core Capability Development

Defense Critical Infrastructure Protection is an optimization and physics-based analysis capability for defending U.S. Defense Critical Infrastructure (DCI), which is integral to national security, especially during adversarial attacks and major natural catastrophes. DCI is dependent on energy infrastructures to ensure effective mission performance; therefore, resilience against disruptions is essential. Here, the analysis capability based on the **InfrastructureModels** software ecosystem enables an understanding of how energy infrastructure resilience can best enable DCI resilience. This analysis is used to determine consequence to DCI missions from disruptions and identify opportunities to improve resilience both inside and outside of Department of Defense facilities.

Contingency and Vulnerability Identification is an optimization and physics-based analysis capability for identifying failures that have worst-case outcomes or are the most likely to have large impacts on energy infrastructure systems. It is enabled by the **InfrastructureModels** software ecosystem and used to identify the vulnerabilities of independent or interconnected infrastructure systems, estimate the worst and average case damage to extreme events, to analyze the resilience of various infrastructures, and develop robust real-time emergency control and detection methods to protect a grid from large contingency events.

This capability is also used to evaluate and identify failure points in plans for achieving the U.S. integrated energy system future and to ensure that resilience is incorporated as an evaluation metric of plans that meet clean energy targets [26]–[28]. This analysis is embedded in Los Alamos' R&D 100 Award winning Multiple Contigency Solver (MCS) [17] (formerly referred to as the Severe Contingency Solver).

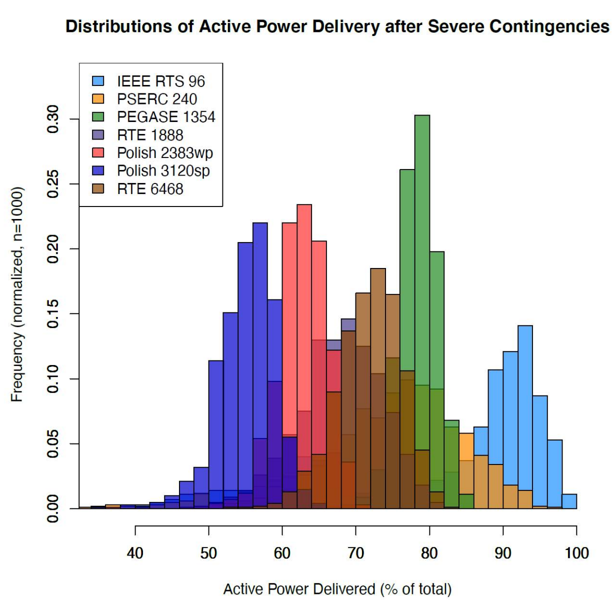


Figure 3-2: Distributions of maximal active power delivery in extreme damage scenarios for seven open-access power transmission networks. The verity of means and variance across the networks indicates that each power network has distinct relicense properties in the multi-contingency regime.

Extreme Event Resilience is an optimization and physics-based capability for analysis of extreme climate events and man-made hazards that threaten energy infrastructures. The **InfrastructureModels** software ecosystem enables the development of a variety of frameworks and tools – including numerical optimization and statistical tools, natural system modeling[8]; algorithms to estimate damage to infrastructures caused by hazards, and the Multi-Contingency Solver [17]; – to model complex artificial and natural systems (e.g., wildfire, severe weather, climate evolution) for identifying events that are of most concern, estimating how these extreme events damage energy infrastructures, and then applying control, mitigation, and optimization to make recommendations on how to limit the impacts of these events.

Restoration Planning is an optimization-based analysis for restoring electrical power transmission and/or distribution networks (either connected to- or disconnected from the bulk energy system) from a de-energized state. **PowerModelsRestoration** (for optimal restoration planning), **PowerModelsDistribution** (for optimal power flow and optimal load shedding), **PowerModelsONM** (for optimal switching and optimal load shedding), and other tools of the **InfrastructureModels** software ecosystem are integrated to support planning, decision making, and implementation activities. This capability could be used to determine a strategy for resilience-based microgrids, distributed energy resource driven blackstart, and segmented restoration anywhere in the U.S.

[8] https://www.frames.gov/firetec

4 Supporting DOE Priorities

This section discusses how Los Alamos' ***Core Capability Development*** may be used to support the DOE's four goals of *Decarbonization*, *Infrastructure Modernization*, *Equity and Energy Justice*, and *Climate Adaptation and Mitigation*. The following sections present example problems in each of these areas that could be addressed with Los Alamos capabilities, demonstrating how we are well positioned to support DOE's priorities.

The R&D structure outlined in Figure 1-1 is designed to support a modular, agile approach to research so that capabilities can adapt to emerging needs. Los Alamos investments in *Fundamentals* over the past decades are aligned with the DOE's goals, and continued advancement in these will remain a priority to sustain the scientific leadership of the DOE. Similarly, the *Implementation*s are core building-blocks for advancing the DOE's goals, augmented by additional blocks under development to meet evolving requirements. Finally, the *Tools* that Los Alamos has developed enable complex *Analysis*, which can immediately support the DOE; with opportunities to develop new tools and analyses on the foundations of *Fundamentals* and *Tools*.

4.1 Decarbonization

Decarbonization is the process of removing carbon dioxide emissions from our energy systems. From a computational perspective, this problem is challenging because it requires new methods for handling uncertainty and variability in energy production and requires significant analysis for assessing the economic viability of new decarbonization technologies.

Example 1: Los Alamos' *Analysis* can support decarbonization through the demonstration and deployment of control approaches for optimized system response (relying on **Infrastructure Investment**, **Infrastructure Simulation**, and **Infrastructure Performance Planning**). These control approaches support the integration of intermittent resources by mitigating the effects of uncertain energy production. Additionally, renewable resources are anticipated to displace fossil fuel-based generation, which requires planning to identify alternative technologies, like storage, to balance intermittency. Here, the analysis Los Alamos provides can assist decision makers in reducing the utilization of fossil fuels, identifying fossil fuel plants to decommission, and recommending technology mixes (new control, storage, etc.) to reduce and eliminate carbon-based generation sources.

Example 2: Some clean energy planning scenarios consider carbon capture or direct air capture to prevent and remove CO_2 from the atmosphere and sequester it underground. Other scenarios consider H_2 as a new fuel source, which when paired with intermittent renewable resources could serve as energy storage and a means to smooth fluctuating, variable energy production. All scenarios are faced with the challenge of transport: how to move CO_2 and/or H_2 from its point of production to its point of storage or use. Over the long-term, pipeline transport is considered to be one of the more economical options. Los Alamos *Analysis* capabilities (**Pipeline Re-purposing Planning**) can assist in analyzing existing pipeline infrastructures and identifying candidates for supporting H_2 production and CO_2 sequestration or planning for the design of a cost effective national-scale H_2 and/or CO_2 pipeline transport system.

Supporting DOE Priorities

4.2 Infrastructure Modernization

Investing in infrastructure improvements, commercializing technologies currently in the RD&D phase, and developing novel infrastructure operational practices are all necessity as energy infrastructures transition to a more decarbonized and resilient future.

Example 1: *Fundamentals* to optimize, control, and learn the complexities of interconnected engineered networks – such as electric power, natural gas, and water infrastructures – and *Tools* developed under the **InfrastructureModels** software ecosystem allow Los Alamos to design resilient infrastructure systems (**Infrastructure Investment**), simulate interdependent network behavior (**Infrastructure Reliability Assessment**), and use advanced integrated control and optimization methods for improved network operation under uncertainty (**Infrastructure Performance Planning**). In addition, related capabilities to model and analyze critical infrastructures (**Defense Critical Infrastructure Protection**, **Contingency and Vulnerability Identification**, and **Extreme Event Resilience**) enable Los Alamos to make recommendations on how to better protect these systems against a variety of natural and man-made threats.

Example 2: Clean H_2 and related technologies – such as electrolyzers, fuel cells, and turbines – play a key role in decarbonizing many sectors, including medium- and heavy-duty transportation, residential and commercial heating, power generation, and hard-to-decarbonize industries such as ammonia and steel. Advanced Los Alamos *Analysis* capabilities (**Infrastructure Investment**, **Infrastructure Performance Planning**, and **Pipeline Re-purposing Planning**) could assist in the development of regional clean H_2 hubs that can demonstrate the production, processing, delivery, storage, and end-use of clean H_2.

4.3 Equity and Energy Justice

Equity and Energy Justice declares that the clean energy revolution must lift up the communities that have been left behind historically, and make sure those who have suffered the most are the first to benefit from federal funding available to support energy transitions.

Los Alamos is committed to, and actively promotes diversity, equity, and inclusion by "*striving to create and sustain an organizational culture and working environment that provides all employees with an equal opportunity to maximize their potential within the context of the Laboratory's mission*" as stated by the "Los Alamos National Laboratory Equal Opportunity, Affirmative Action, and Diversity" program. One example of how Los Alamos' efforts in social equity impact R&D in infrastructure modeling is discussed next.

Example: Los Alamos *Analysis* capabilities can meaningfully contribute to national policy discussions, including specific studies and/or white papers prepared for federal and state government agencies to construct collaborative communities. An example of this is the biennial LANL Grid Science Winter School & Conference, which addresses DOE's priority to engage communities in achieving a just and equitable energy transition.

4.4 Climate Adaptation and Mitigation

Climate Adaptation and Mitigation is the process of reducing emissions of- and stabilizing the levels of heat-trapping greenhouse gases in the atmosphere and adapting current climate change induced conditions.

Example: A changing climate leads to increasingly unpredictable extreme weather events, which pose a growing threat to energy infrastructure systems. The advanced *Analysis* capabilities at Los Alamos enable modeling and analysis of these hazards and their impact on independent, interdependent, and interconnected infrastructures (**Infrastructure Reliability Assessment**, **Contingency and Vulnerability Identification**, and **Extreme Event Resilience**). With increased understanding of these hazards, advanced tools (such as **PowerModelsRestoration**, **PowerModelsGMD**, and NeSMA framework[9]) and capabilities (**Operation Planning** and **Restoration Control Optimization**) can help estimate future climate and weather threats, assess and mitigate adverse impacts, inform optimal adaptation planning activities, and restore normal operation of infrastructures.

[9] https://www.lanl.gov/projects/nesma

5 Selected DOE Projects

5.1 [ARPA-E] Grid Optimization Competition

Los Alamos Team: **Carleton Coffrin** and Robert Parker
Timeline: FY2019 – present

Challenge:
ARPA-e's Grid Optimization (GO) competition has sought to build the next generation of power systems software by holding an open competition with prize money on the order of $1,000,000 dollars. Modeled after DARPA's "grand challenge" program, the GO competition has brought together the world's best researchers, has provided a consistent computational platform for rigorous benchmarking of emerging power grid algorithms, and has pushed researchers to solve problems at industry-relevant scales. The first three iterations of the GO competition have focused on AC security constrained optimal power flow (SCOPF), a non-convex nonlinear optimization problem with billions of decision variables and constraints on realistic power network datasets. The competitors are tasked with building optimization software that can reliably solve these problems in 10 minutes or less.

Technical Approach:
Los Alamos leveraged its world-leading expertise in nonlinear optimization for optimal power flow (OPF) to develop novel SCOPF algorithms for solving the G) competition problems. With the SCOPF problem specification spanning over 100 pages and the software required to run in a distributed computing setting with six computers working in parallel, Los Alamos' competition algorithms are extremely sophisticated and demonstrate a high technology readiness level (TRL) that is ready for industry adoption and serve as the reference solution for the competition.

After the conclusion of each competition, all of Los Alamos' software for solving these challenging problems was made open-source as part of the **InfrastructureModels** software ecosystem, which has benefited the research community and commercial software developers by showing how Los Alamos' research can be deployed as reliable and performant grid optimization algorithms In the first GO competition (2020), Los Alamos staff took two out of the top 10 positions, with one team making it to the top 5. In the second competition (2021), Los Alamos staff won the first and second place in the leaderboard corresponding to the Trial 1 event.

Impact:
Given that modern power markets clear billions of dollars annually, even small improvements in efficiency (on the order of 1%) can save the United States hundreds of millions of dollars annually. The GO competition seeks to build a new generation of optimization algorithms that leverage recent developments in nonlinear optimization to improve the efficiency of the grid while ensuring reliability. To that end, the competition provides its competitors with a computing environment that accurately replicates the conditions of modern grid operating rooms and demonstrates that the proposed algorithms are ready for a realistic production setting.

5.2 [AGM] Grid Science Winter School and Conference

Los Alamos Team: **Russell Bent**, Adam Mate, Harsha Nagarajan, Kaarthik Sundar, and Deepjyoti Deka
Timeline: FY2015 – present

Challenge:
The problems and challenges, faced by the energy systems community, have grown increasingly complex over the past decades; solutions require multi-disciplinary approaches, expertise, and education.

Technical Approach:
The Los Alamos *Grid Science Winter School and Conference* series covers theoretical and algorithmic aspects of energy systems that have immediate and potential future importance to the research community. Areas of focus have been wide-ranging, drawn from emerging theoretical needs perceived within the DOE OE, including: ethics in AI and ML, resilience, distribution network modeling, and interdependent infrastructures. These needs are challenging crosscuts between related, often isolated research areas, including computation, control, optimization, and analysis.

Figure 5-1: Class of 2023 Grid Science Winter School.

Each event lasts for five days: three days of Winter School, followed by two days of Conference. The Winter School portion consists of 9 lecture blocks – each 60-90 minutes block represents a single subject – given to roughly 30-40 graduate students and postdocs, chosen via an application and screening process to ensure high-quality attendees who are able to extract the maximum possible from the opportunity. The lectures introduce the students to a range of advanced theoretical topics that are not typically available at their home institutions, and provide in-depth discussions of examples to give a more solid understanding of the introduced approaches. The intent is not to make the students immediately able to apply the theoretical techniques, but rather to demonstrate the usefulness of the methods, stimulate interest in them, and develop crosscutting collaborations between students from different disciplines. The Conference portion consists of presentations by established and emerging top researchers in theoretical methods applied to energy systems; robust discussion and debate of topics is encouraged. Each student attendee of the Winter School is required to present a poster and a committee of judges awards a "Best Poster" prize.

Impact:
New models and algorithms, sought by the DOE OE Advanced Grid Modeling (AGM) program, cannot be developed in a vacuum and, once developed, should not reside in a vacuum. The *Grid Science Winter School and Conference* series builds interdisciplinary collaboration with experts in related fields and brings their expertise and insights to the research while ensuring that the models and techniques developed are beneficial and useful to the wider community. This event enables both the dissemination of these results and the creation of a highly skilled workforce needed to transform energy systems to deal with the major challenges of the next several decades.

5.3 [AGM] Robust Real-Time Control, Monitoring, and Protection of Large-Scale Power Grids in Response to Extreme Events

Los Alamos Team: **Yury Maximov**, Deepjyoti Deka, and Wenting Li
Timeline: FY2020 – FY2022

Challenge:

The protection and emergency control system for the US transmission grid is one of the most crucial national security points. Increased variability in the system state due to a higher level of renewables and frequent extreme weather events leads to greater demand and diversity in the required control actions than traditional schemes. The project has designed a new generation of controls that integrates with existing automated and manual protection and operational processes while also allowing these processes to continue operating. The new emergency controls include fully automated, real-time corrective actions to ensure voltage and transient stability following a significant disturbance. The controls take the system from a post-disturbance emergency state to a stable restored state so that the system operator may confidently resume normal, economically optimized operations. The emergency control actions are computed in real-time, making them adaptive to the current system state and the imposed disturbance.

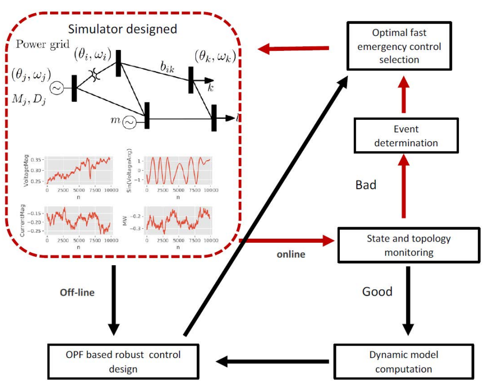


Figure 5-2: Emergency control operation pattern in a power grid. The project contributes both real-time detection and mitigation of an extreme event.

Technical Approach:

By designing novel numerical optimization and statistical tools to address non-convex problems, Los Alamos was able to reformulate AC power flow in a computationally efficient form to enable real-time computations of control actions. Our steady-state algorithms outperform more traditional undervoltage load shedding schemes in providing stabilizing control actions and accurate predictions of the post-contingency operating point. We further adapted the methods to ensure dynamic stability of the system using frequency regulation, HVDC power injections, SVC reactive power injections, and load shedding as controls. The proposed methodology has recently been extended to efficiently model cascading processes by constructing a proxy for the impact of cascading events and further incorporating it to the emergency control optimization problem to optimize over both the preemptive and corrective response to large disturbances. The algorithms were published in multiple IEEE Transactions on Power Systems papers and are partially implemented in DOE supported software DCAT and GridDyn.

Impact:

The project's primary impact is robust real-time emergency control and detection methods that incorporate AC power flow physics and non-linear dynamics to protect a grid under large disturbances, such as a significant contingency or an extreme weather event. It is now possible to rapidly detect an extreme event and identify proper corrective actions in a similarly short time-frame to mitigate the associated risk, which leads to revisiting traditional RAS/SPS based control response. Our team member, Prof. Wachter, was awarded the second prize at the DOE Grid Optimization Competition for the contribution to security-constrained grid optimization.

Selected DOE Projects

5.4 [AGM] Hybrid Learning Assisted Optimization Methods for Uncertainty Management and Corrective Control

Los Alamos Team: **Sidhant Misra** and Marc Vuffray
Timeline: FY2020 – FY2022

Challenge:
Preventive and corrective controls are necessary for uncertainty management and to ensure safe and economic operations under uncertainty. An adjustable robust optimization (ARO) formulation built around the optimal power flow that incorporates preventive and corrective controls can produce the most efficient control actions and dispatch set points. However, due to significant computational burden, currently a limited number of preventive measures such as N-1 security, and corrective measures such as AGC and AVR are incorporated into optimal power flow formulations, and as such these formulations are already quite challenging.

Technical Approach:
This project has developed learning assisted optimization techniques for efficient and reliable uncertainty management and decision making at faster time scales. By leveraging recent advances in machine learning, the data available from load and uncertainty forecasts, from routinely solved optimal power flow and, synthetic data generated from offline computations has been used to inform and significantly boost current and new optimization tools used in operations. This provides a flexible and comprehensive optimal power flow (OPF) based ARO framework that incorporates preventive and corrective actions and accommodates current and potential future practices. The methods leverage recent advances in active-set learning for constrained optimization to identify critical constraints and thus reduce complexity. These learning tools are used for generating advanced non-linear corrective control policies for more efficient utilization of available corrective control resources by utilities.

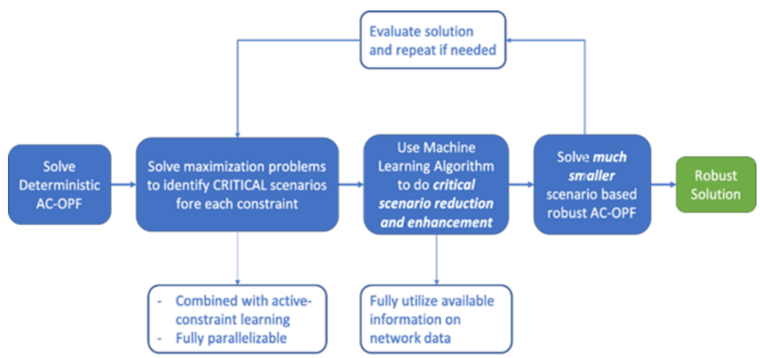


Figure 5-3: Data-driven scenario selection and enhancement algorithm process flow.

Impact:
Given that most power system tools for determining generator dispatch incorporate limited requirements on reliability and resilience, this approach supports a wider suite of security constraints to be incorporated in formulations like optimal power flow and account for system response during extreme conditions such as preventive actions and corrective control actions. This limits reliance on ad-hoc policies and reduces the need to resort to expensive emergency controls and improve economic efficiency.

5.5 [AGM] Weather Outage Prediction Model

Los Alamos Team: Donatella Pasqualini
Timeline: FY2019 – present

Challenge:
To date, there is no comprehensive model to describe how hazardous weather events of different types impact the electrical grid, with most work focused on hurricanes. The challenge in developing a comprehensive model for situational awareness is due to the difficulty of identifying extreme weather events that are not hurricanes. While quantifying impacts from tropical cyclones can easily be done both spatially and temporally, identifying winter storms is much more difficult. They are less predictable, less well spatially and temporally defined, and have more localized and diverse impacts than tropical cyclones. In addition, most of the existing models are customized for specific regions and power distribution systems and there is not model that can operate at national scale.

Technical Approach:
Our approach leverages existing capabilities developed for hurricane induced outages and the experience of our collaborators at the University of Connecticut and develops a new workflow that (1) identifies weather events that may damage the power system and (2) forecasts the geographical distribution of power outages. The effort employs climatic and weather-related data from the National Oceanic and Atmospheric Administration (NOAA) and historical power outages to train a statistical power outage forecasting model. The final deliverable of this effort is a decision-support tool that the electrical power utilities can use to forecast areas at risk for power outage.

Impact:
Under prior work, Los Alamos has supported the Department of Homeland Security's National Infrastructure and Simulation Analysis (NISAC) program by developing a set of statistical models, e.g., Electrical Power Outages Forecast models (EPoF), to predict at national scale electrical power outages due to hurricanes. EPoF uses the state-of the-art statistical approach to forecast at national scale outages requiring as inputs a larger set of publicly available parameters. As a real-time situational awareness and emergency and mitigation planning tool, Los Alamos deployed EPoF as an automated workflow within a Web based geospatial visualization environment that is used by DHS to respond to extreme events. For DOE, this capability has been extended to support emerging OE outage prediction needs for extreme weather like ice and cold weather storms.

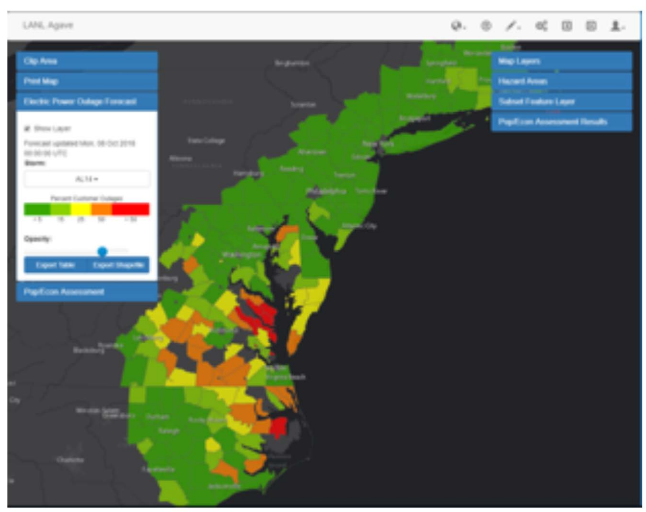


Figure 5-4: AGAVE, AWS cloud-based, Web application for real-time hurricane electrical power outages forecast.

Selected DOE Projects

5.6 [AGM] Optimized Resilience for Distribution and Transmission Systems

Los Alamos Team: **Russell Bent**, Andreas Wachter, David Fobes, and Juan Ospina
Timeline: FY2021 – present

Challenge:
Transmission and distribution systems have traditionally been owned and operated by separate entities, largely due to a lack of active controls in the distribution network. Historically, a transmission operator could operate without detailed information or coordination with distribution operators. However, the past several years has seen incredible rises in active resources on distribution feeders like distributed energy resources (DERs), demand response (DR), microgrids, and other controllable technologies. This rise has yielded both challenges and opportunities that are difficult for industry to address without comprehensive wholistic modeling of both systems simultaneously. Therefore, the development of a single formulation for modeling joint transmission-distribution optimization problems, creating a basis for joint resource management and dispatch that goes far beyond scenario-driven, co-simulation methods, is critical for efficiently and reliably operating modern grid systems.

Technical Approach:
We have developed algorithms to find optimal operating conditions, using relaxation and approximation methods to obtain guarantees about those optimal conditions. The key approach is a combination of mathematical formulations, e.g., approximating the power flow physics to quickly obtain feasible bounds, and using those bounds to obtain optimal AC solutions. We leverage the large body of open-source optimization tools developed at Los Alamos, including **PowerModels** and **PowerModelsDistribution**, which separately model the power flow physics of transmission and distribution systems, respectively. We developed prototype algorithms based on these tools and tested them on transmission-distribution models of increasing complexity and size, building up to an ISO relevant problem including distribution resources to improve the response of the bulk electric system during an extreme event. The anticipated outcome is a demonstration of how using distribution network resources improves the overall resilience of a transmission system during such events. The project includes a collaboration with Northwestern University that promotes workforce development in this strategic area.

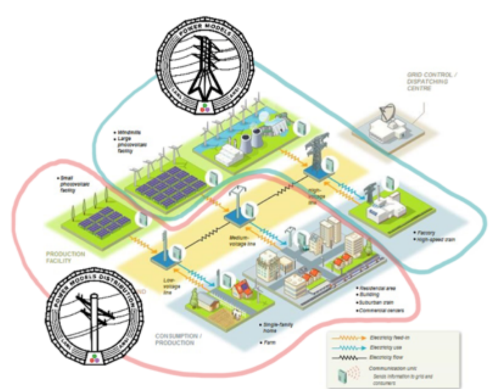


Figure 5-5: Power grids are typically separated into two categories in modeling: 1) transmission, which are generally treated as single-phase positive sequence networks, representing the bulk of all generation, and serving large industrial customers, and 2) distribution, which are more accurately unbalanced multiphase networks that serve medium to small customers and representing comparatively less generation than transmission.

Impact:
Advanced system co-optimization theory, methods, and tools are needed to provide system planners and operators with cross-domain visibility of system conditions and constraints. Without these advancements to optimization-based coordination, future deployments of controllable technologies in distribution networks could increase the possibility of coupled system collapse, especially during extreme events.

5.7 [AGM] Space Weather Mitigation Planning

Los Alamos Team: **Arthur Barnes**, Adam Mate, and Russell Bent
Timeline: FY2023 – present

Challenge:
Geomagnetic disturbances (GMDs), resulting from intense solar activity caused by coronal mass ejections, pose risks to the electric grid by generating geomagnetically induced currents (GICs) through interaction with the Earth's magnetic field, resulting in the flow of ionospheric electrojet sources. The resulting time-varying fields generate currents within the earth, resulting in surface electric fields that couple into transmission lines, which in turn causes quasi-dc GICs to flow through those lines. The GICs modify the ac behavior of transmission network by causing half-cycle saturation of transformers, drawing harmonic currents and a net increase in reactive power consumption.

To protect against these threats, dc-current blocking devices may be included into the network. These blockers, however, are expensive; additionally, dynamic measures to deal with GICs include controls, such as generator dispatch, load-shedding, and line switching. Developing a GIC-aware optimal power flow (OPF) that includes ac physics, transformer reactive losses, small-signal stability etc., is a challenging computational problem for the community and requires advanced algorithmic techniques.

Technical Approach:
This project integrates the individual elements developed by past Los Alamos projects into a planning problem formulation that supports the placement of dc-current blocking devices to mitigate the effects of GICs on the bulk electrical system (BES). This complete formulation creates the basis for resilience planning based on uncertainty associated with future GIC, the dynamics of the GIC events over time, and the combined physics of ac power and GIC. The project is developing novel prototype algorithms tested on BES GIC models of increasing complexity and network size and building to an ISO relevant optimal planning problem. It also includes a unique partnership with the DOE Office of Science, leveraging the expertise and technology of the "Scientific Discovery through Advanced Computing" (SciDAC) centers.

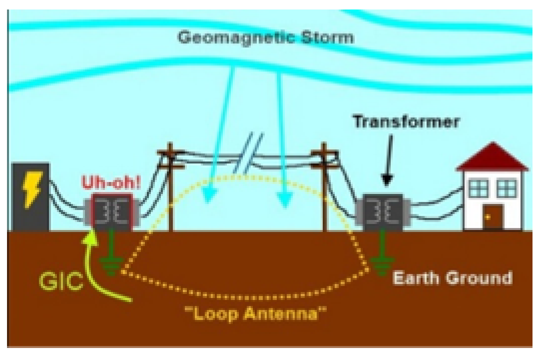


Figure 5-6: Schematic of interactions between power systems and geomagnetic storms.

Impact:
When GMDs occur on large energy systems, the resulting power outages may be catastrophic. For example, the 1989 event in Quebec led to the shutdown of the Hydro-Quebec system, as a consequence 6,000,000 people suffered power outage for nine hours; a report estimated that the net cost of this event was $13.2 million, with damaged equipment accounting for $6.5 million of the cost. Potential GMD impacts to transformers motivate research that will improve our understanding of such events and identify strategies to mitigate impacts. Without these advancements to optimization-based planning, future infrastructure designs are vulnerable to GIC induced voltage collapse and transformer failure, which this project seeks to address.

Selected DOE Projects

5.8 [NAERM] North American Energy Resilience Model

Los Alamos Team: **Russell Bent**, David Fobes, Mary Ewers, Kaarthik Sundar, Adam Mate, Anup Pandey, James Wernicke, Anatoly Zlotnik, Shriram Srinivasan, and Sai Hari
Timeline: FY2019 – present

Challenge:
The Nation's energy resilience is dependent on an ability to provide national-scale energy planning and real-time situational awareness. While each energy domain has some capability to support such national-scale modeling, given scalability and other barriers, there was not a DOE modeling capability that could span interdependent energy domains. The North American Energy Resilience Model (NAERM) was developed to provide such a capability to the Nation and ensure reliable and resilient delivery of energy across multiple energy sectors.

Technical Approach:
The overall technical approach of NAERM is to bring together the best capabilities and resources of eight national laboratories to build a software platform that supports co-simulation and analysis of the North American energy system. Los Alamos is supporting this effort by providing natural gas modeling and analysis expertise in collaboration with Argonne National Laboratory, leadership in validation, verification, and uncertainty quantification, and methods for identifying critical components in energy systems. This includes integrating Los Alamos' natural gas modeling software, **GasModels**, into the HELICS co-simulation platform and the broader NAERM software system.

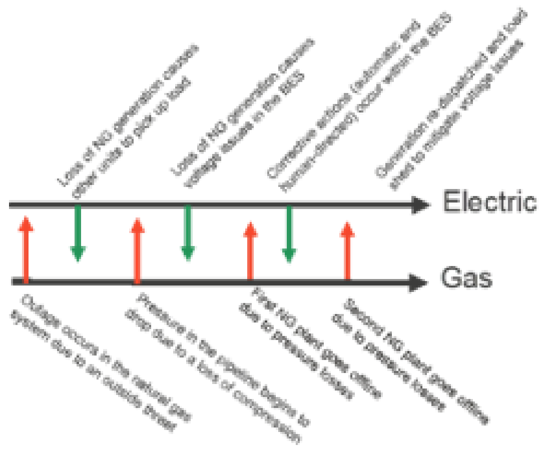


Figure 5-7: A schematic of the types of co-simulation resilience use cases NAERM is designed to model.

Impact:
NAERM supports DOE's provision of situational assessment advice to industry and government. This advice is intended to ameliorate the risk of and consequence of large-scale service disruptions between infrastructure domains. The NAERM is advancing the state-of-science in planning and operations of energy supply during extreme events and provide rigorous resilience and associated economic metrics for these sectors.

5.9 [GMLC] Energy Resilience for Mission Assurance

Los Alamos Team: **Mary Ewers**, Anatoly Zlotnik, Shriram Srinivasan, and Sai Hari
Timeline: FY2022 – present

Challenge:
Defense Critical Infrastructure (DCI) is integral to United States national security, especially during major catastrophes both natural and manmade. Furthermore, DCI is dependent on energy to ensure effective mission performance, so a resilient gas and power grid is essential for national security. Currently, there are no widely accepted quantifiable metrics that adequately reflect the consequence to DCI missions from disruptions to the gas and power grids. This project answers the question: to what degree does weak resilience of the gas and power grids impact DCI mission space and what are realistic opportunities to improve that resilience both inside and outside of Department of Defense (DoD)-owned facilities?

Technical Approach:
Los Alamos extended the **GasModels** software, a network contingency analysis capability for calculating expected gas outages, to include coupled steam and hot water distribution systems. Los Alamos created a **ThermalModels** model based upon the **GasModels** and **WaterModels** formulations, and includes the interdependency between power, gas, and thermal systems. Los Alamos supported a use case to model the resilience of the coast guard facility on Kodiak Island, Alaska.

Impact:
The near-term impact of this project is a demonstrable improvement in a DCI facility's ability to understand how grid resilience can improve their resilience. By advising NAERM in using these metric formulations within their models, an additional impact has improved consideration of DCI needs within investment planning and real-time awareness at the transmission level.

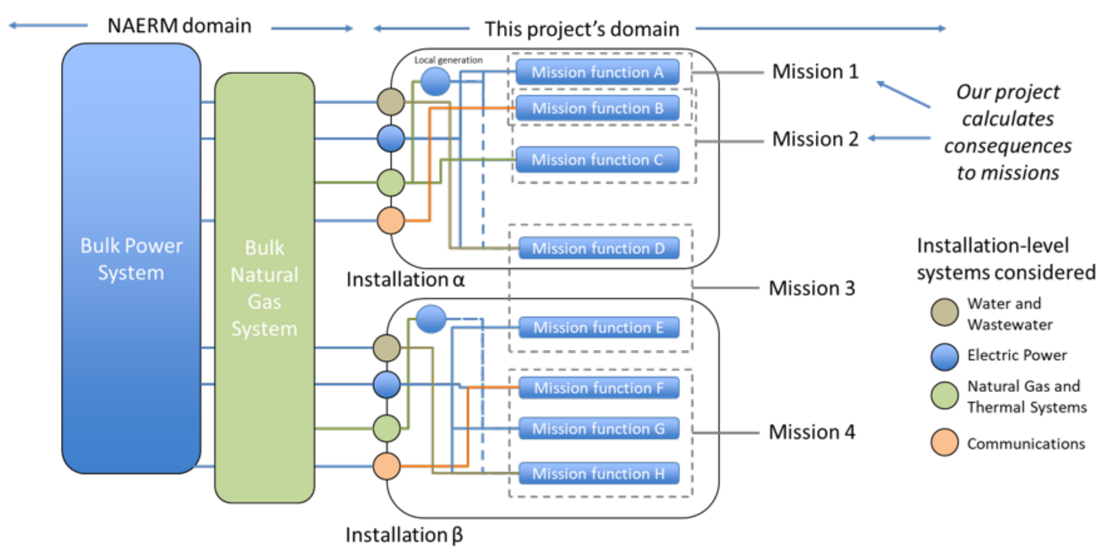


Figure 5-8: Relationship of bulk system performance to the performance of missions and DCI. This figure shows the clean handoff between the NAERM focus and this project's focus.

5.10 [MRD] Resilient Operations of Networked Microgrids

Los Alamos Team: **Russell Bent**, David Fobes, Carleton Coffrin, Arthur Barnes, Jose Tabarez, Hassan Hijazi, Harsha Nagarajan, Smitha Gopinath, and Haoxiang Yang
Timeline: FY2020 – FY2022

Challenge:
The Nation's distribution utilities have access to engineering tools for system planning and operation; however, these tools have some notable limitations: they do not offer the ability to model extreme event damage, they cannot accurately model microgrid capabilities and control options, and they cannot provide optimization-based design solutions. While past work at DOE has led to capable microgrid design tools, optimal resilient design tools, and recovery tools, separately these capabilities do not comprehensively consider the abilities of networked microgrids to dynamically interconnect and share load. In particular, existing microgrid design tools are unable to model the potential value of supporting loads outside the boundaries of the microgrid, the resilient design tools do not model reconfigurations that combine and expand microgrids to form powered islands, nor do they provide detailed generation mixes and feasible control methods, and the recovery tools do not account for changes to the distribution system that would improve recovery activity performance.

Technical Approach:
RONM's multi-lab technical approach includes three capability development activities and one outreach and deployment activity: 1) Formulation and Methodology which develops the formulation for resilient reconfiguration algorithms and restoration algorithms and adds first-of-kind advanced engineering objectives and constraints on system stability, device protection, regulatory restrictions, and economic considerations; 2) Software Implementation, which develops and implements a scalable algorithm for solving the problem formulated in previous activity; 3) Evaluation and Demonstration, which uses distribution system models – adapted from a test system provided by the National Rural Electric Co-op Association (NRECA) and from a system model provided by IOU partner San Diego Gas & Electric – to evaluate RONM solutions for reconfiguration and restoration of distribution systems after extreme events, during which solutions are first verified using software simulation and second validated on a sophisticated HIL evaluation platform; and 4) Deployment and Outreach, which deploys the RONM software on NRECA's Open Modeling Framework platform for use and delivery to the Nation's distribution utilities.

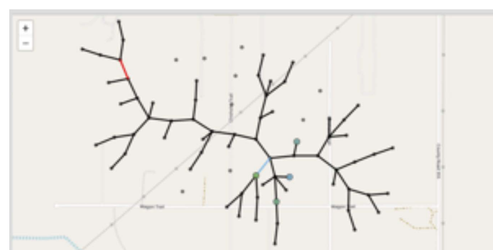


Figure 5-9: RONM map interface that gives a visual representation of the feeder system with microgrids. The interface shows the faulted line (an input) as red and items on the recovery timeline. Items are color-coded based on the time at which they occur (bluer is earlier and greener is later).

Impact:
As extreme event damage to the electric grid continues to grow, it is clear that there is a critical need for an advanced resilience tool such as RONM. Recovery is becoming increasingly more challenging, therefore, utilities must learn how to adapt their approaches to incorporate advanced technologies like inverter-based generation and storage and provide support to defense-critical infrastructure for longer term supply and resilience. Deployment of microgrids can address these challenges by providing backup power and controllable resources for black start restoration.

5.11 [MRD] MgRavens

Los Alamos Team: **David Fobes**, Russell Bent, Harsha Nagarajan, and Jose Tabarez
Timeline: FY2023 – present

Challenge:

In an ideal world, computational modeling to support the planning and design of microgrids would be completely modular; it would give users, from researchers to utilities, the ability to seamlessly pick-and-choose their preferred model for each piece of the process. Current state-of-practice in microgrid planning and design tools has yet to meet this aspirational state, and this project seeks to address this challenge. The realization of this goal is complicated by the observation that planning and design processes are different for each user, meaning that software composability and data exchange is critical for aiding in the creation of custom workflows specific to each user's use case and is the key enabling paradigm of this project.

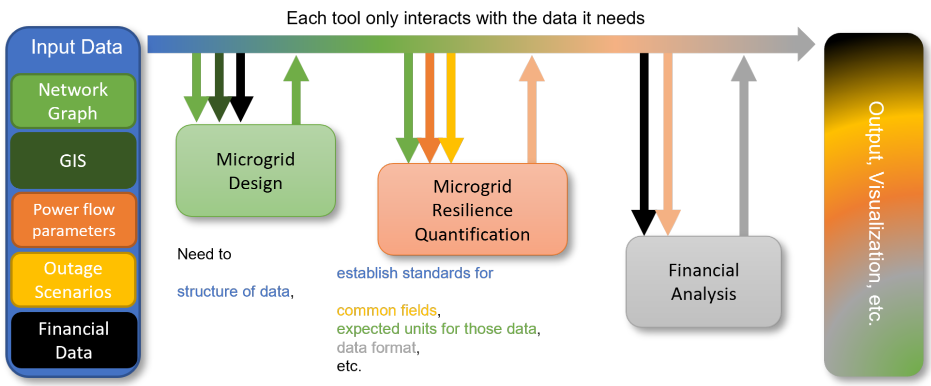


Figure 5-10: MGRavens schematic of use case inspired interoperable and composable workflows for supporting microgrid investment and operational planning.

Technical Approach:

MgRavens tackles the problem of solving data interoperability to achieve improved software modularity in the microgrid modeling arena by developing a core data Application Programming Interface (API) for a particular set of use cases. The improved modularity will be demonstrated by deploying tools on an open-source and free-to-access planning and management framework – the Open Modeling Framework[10], maintained by the National Rural Electric Cooperative Association – available to utilities for modeling, followed by testing and incorporating feedback by a user group directed by a governance board composed of developers at the laboratories, from universities, and from utilities and industry.

Impact:

By investing in software standardization, the DOE Microgrid program and the MgRavens provides its considerable history of capabilities to a broader audience by removing hurdles to technology adoption by stakeholders. This project also specifically impacts the DOE goals in clean energy and energy justice by defining microgrid design use cases that consider social vulnerability metrics in the design phase and evaluate the resilience benefits using the microgrid planning tools.

[10] `https://omf.coop`

Selected DOE Projects

5.12 [DOE] Intermountain West Energy and Sustainability Transitions

Los Alamos Team: **Melissa M. Fox**, Jolante W. van Wyjk, Rajesh J. Pawar, and Kevin D. John
Timeline: FY2021 – present

The U.S. has set a target to reach carbon neutrality economy-wide by no later than 2050, which means carbon dioxide emissions must drop at the gigaton-per-year scale. This will require significant changes in how we produce and consume energy. Thoughtful planning for such a transition takes time, but many communities throughout the Nation are already facing economic and environmental challenges related to energy transition. This is especially true for coal, oil and gas, and power plant communities that have fueled the nation's prosperity for decades.

A Region in Transition

In 2021, the DOE funded the Intermountain West Energy and Sustainability Transitions (I-WEST) initiative as a pilot effort to scale down national energy goals to a regional level to better understand what energy transition means in terms of local economies, natural resources, infrastructure, workforce, and technology acceptance. The six states included in the I-WEST initiative -— Arizona, Colorado, Montana, New Mexico, Utah, and Wyoming —- are all characterized by fossil fuel-based economies and have shared challenges related to climate change. As major producers and exporters of fossil-based energy, these states are highly vulnerable to social and economic disruptions because of energy transition, but also have many advantages that could position them as emerging leaders in new energy economies.

One of the overarching strategies of I-WEST is to build a regional team to assess the energy landscape, identify pathways to build symbiotic energy economies, and recommend solutions to the challenges energy communities are facing. Each state is represented in the initiative by a local college, university, or national laboratory. Additional partners from beyond the region were selected for their expertise in applicable fields.

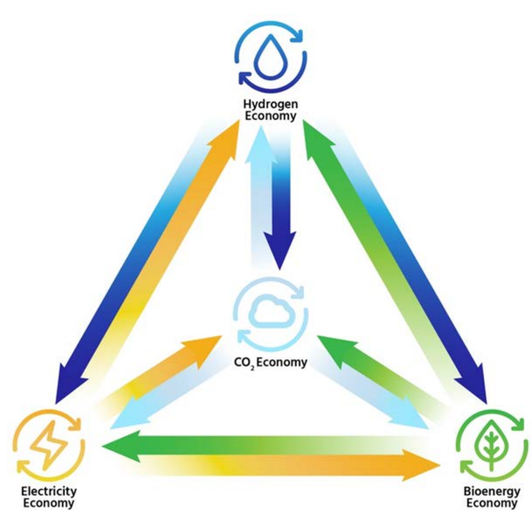
A Place-Based Approach and Why it Matters

The amount of federal funding currently available for clean energy research and infrastructure development is unprecedented, but the success of programs funded by these dollars rests on effective planning and implementation at the local level. I-WEST takes a place-based approach that considers the specific circumstances of the region and engages communities to actively participate in decisions that will affect them in the long term. Additionally, I-WEST takes a technology-neutral approach that prioritizes societal readiness first and technology readiness second. This is a departure from the traditional approach to developing new energy systems, in which regional perspectives are often not factored into the equation until after decisions have been made, and those decisions are based primarily on the maturity of a technology.

Through I-WEST, a collaborative network of tribes, public servants, policy makers, researchers, educators, advocacy groups, and business leaders come together to share information at workshops, seminars, symposia, listening sessions, and other events to network, exchange information, and share lessons learned. These events yield valuable input that is integrated into the I-WEST roadmap. Perhaps even more importantly, these engagements help establish communication channels between stakeholders—a critical step toward building regional coalitions that can work together to implement the I-WEST roadmap.

Symbiotic Energy Economies

Leading experts in climate and energy sciences, such as the Intergovernmental Panel on Climate Change, recognize that achieving carbon neutrality will require multiple pathways. Moreover, they recognize that those pathways must not only result in reduced greenhouse gas emissions, but they also must be sustainable. Putting both principles into practice, the I-WEST roadmap considers four symbiotic "economies" that could be exploited to decarbonize critical energy sectors in the Intermountain West, while simultaneously building new industries that leverage the region's infrastructure, workforce, and natural resources. The analyses conducted by I-WEST explore supply-and-demand scenarios for energy based on carbon capture, storage, and utilization; low-carbon hydrogen; bioenergy; and low-carbon electricity. Water usage is also considered a cross-cutting factor, including the potential for leveraging produced water to improve efficiencies.



These four economies are distinct yet symbiotic and highly dependent on one another from a supply and demand perspective—the growth of each depends on the co-development of all the others. As one of many examples, captured carbon dioxide (CO2) can be used with green hydrogen to produce sustainable, carbon-neutral chemicals and fuels as replacements for petroleum-based products. The symbiotic nature of these economies has the potential to accelerate development, but could also result in competition for infrastructure, natural resources, and workforce, which could slow growth. This emphasizes the need for an I-WEST roadmap as a tool to help communities evaluate the risks and opportunities associated with new energy technologies.

Selected DOE Projects

Stakeholder Outreach

Building relationships with energy communities through continuous stakeholder outreach is a central tenet of I-WEST. In addition to hosting workshops, listening sessions, and seminars the I-WEST website is another important tool for staying connected with stakeholders. Developed for a broad audience with diverse backgrounds and areas of interest, the website is a platform to both inform and hear from stakeholders with a vested interest in energy transition in the Intermountain West. It houses an interactive catalog of energy projects across the region (organized by technology pathway), a newsfeed with articles and blogs, announcements about upcoming events, and a timeline of past events with links to published resources like videos, slides, and reports.

Next Steps

Outcomes from the first 18 months of I-WEST are published in an online report that provides an overview of the initiative, key findings, and recommendations for next steps in energy transition planning, as well as a nascent roadmap that serves as a foundation for future case studies, analyses, and stakeholder outreach. The DOE energy programs are providing guidance on future directions of I-WEST, particularly areas in which more in-depth analyses are needed to inform technology development, deployment, and demonstration initiatives.

6 Partnerships and Pipelines Office

The **Partnerships and Pipeline Office (PPO)** at Los Alamos National Laboratory is designed to make science, technology and engineering collaboration and recruitment possible by providing key resources needed for these efforts.

FEYNMAN CENTER FOR INNOVATION

The Feynman Center drives Los Alamos innovation as an essential part of our national security mission by accelerating connections between research, corporate, and entrepreneurial communities; building partnerships and mechanisms that deliver our technology to solve our Nation's biggest challenges; and creating a trusted external network to extend and enhance our Laboratory's ability to meet core mission. The Feynman Center facilitates the process of putting agreements in place to enable collaborative work between Los Alamos researchers and partners from industry, academia, and the broader research community. Many projects at Los Alamos sponsored by the **DOE Energy Programs** encompass work supported by Cooperative Research and Development Agreements (CRADA), Non-Disclosure Agreements (NDA), Strategic Partnership Project (SPP) Agreements, Intellectual Property Management Plans (IPMPs), which help spur the commercialization of laboratory-developed technologies.

ENTREPRENEURSHIP FOR MISSION INNOVATION

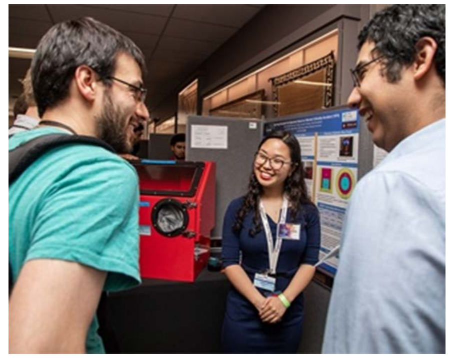
The Entrepreneurship for Mission Innovation (EMI) program integrates entrepreneurial training programs inside and around the Laboratory. EMI fosters an innovative mindset for staff through workshops, funding opportunities, collaborative efforts, and technology accelerator programs. Programs are leveraged for synergy with other indirect funds and enhance collaborative efforts in which Laboratory staff and capabilities can contribute to regional technology vitality. The FY23 Technology Evaluation Demonstration (TED) funding opportunity, managed by EMI, prioritized the demonstration of technologies or methods to address challenges in **Energy Security** with a focus on technical evaluations that accelerate progress toward establishing testbeds and partnerships for **Energy Transition** in the Intermountain West.

NATIONAL SECURITY EDUCATION CENTER

The National Security Education Center focuses on collaborations for education, strategic research, and student opportunities. Its Strategic Centers support a broad spectrum of interdisciplinary science that underpins the Los Alamos' mission in national security. Collaborations established through the Centers provide Laboratory programs with a systematic infusion of new ideas, people, and contact with the larger academic community.

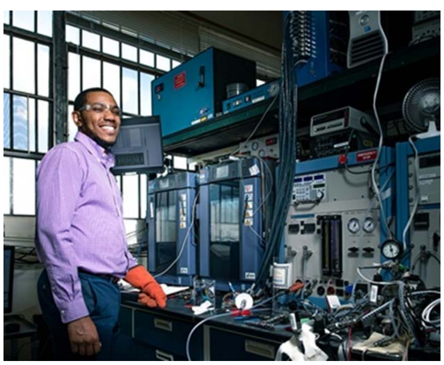
Partnerships and Pipelines Office

STUDENT PROGRAMS



The Student Programs Office supports a variety of educational internships programs to further the Laboratory's strategic goal of developing and mentoring the next-generation workforce of scientific and technical professionals. Los Alamos offers technical and non-technical internships to high schools, undergraduate, and graduate students. A Student Programs Advisory Committee, composed of staff members, students, and postdocs, monitors the quality impact of student programs to ensure effective communication about student programs and recommend policy changes and initiatives for improvement in student programs. The Student Programs Office also supports several special internship programs funded by DOE program offices and extramural agencies such as the NNSA, National Science Foundation, and various colleges and universities. As an example, Los Alamos currently has seven students from Navajo Technical University working on **Energy** projects related to fuel cell manufacturing that are supported by the NNSA Minority Serving Institutions Partnership Program (MSIPP).

POSTDOC PROGRAM



The Postdoc Research program offers the opportunity for appointees to perform research in a robust scientific R&D environment, present and publish research, advance knowledge in basic and applied science, and strengthen national scientific and technical capabilities. There are several types of appointments – Postdoc Research Associate, Fellow, and Distinguished Fellow – all of which are funded through the LDRD program to ensure research appointments are tightly aligned with the Laboratory's science and technology strategy. Fellows are selected based on academic and research accomplishments, the strength of the proposed research, as well as their potential impact at the Laboratory. Distinguished Fellows must display extraordinary ability in scientific research, potential to impact Laboratory programs and/or ability to establish new capabilities and show clear promise of becoming outstanding leaders. Many Los Alamos scientists and engineering contributing to **DOE Energy Programs** were recruited through this program.

DIVERSITY, EQUITY, AND INCLUSION

At Los Alamos, diversity, equity, and inclusion promote innovation, enhances problem-solving, and makes the Laboratory a more successful and productive organization. These principles are essential to how the Laboratory develops teams, conducts its work, and how staff ultimately come together to solve problems of the utmost significance. Los Alamos is recognized annually as a "top employer" or "best place to work" by several organizations. Still, there is more work to be done, and the Laboratory has numerous Employee Resource Groups to help attract, recruit, and retain representative group members.

2022 RECOGNITIONS FOR DIVERSITY

Family-Friendly New Mexico Award (Platinum)
Top 20 Government Employers-Careers and the Disabled (#7)
Top 20 Government Employers-Minority Engineer (#8)
Top 20 Government Employers-Equal Opportunity (#8)
Best of the Best Award: Top Government and Law Enforcement Agencies for Hispanics
Best of the Best Award: Top Government and Law Enforcement Agencies for Women
Top 20 Government Employers for Women Engineers (#9)
Top 20 Government Employers for STEM Workforce Diversity (#17)
50 Best Companies for Latinas (#33)
HIRE Vets Medallion Program (Gold)
Best of the Best Award: Top Government & Law Enforcement Agencies, Black EOE Journal
20 Best Research Companies to Work For (#2)

Appendix A: Developed Computational Solvers

This appendix introduces and describes **Advanced Computational Algorithms** released by Los Alamos as open-source software, which provide a foundation for the advanced analysis and support that the Laboratory provides to the DOE.

Juniper[11] – (**Ju**)mp (**n**)onlinear (**i**)nteger (**p**)rogram solv(**er**) – is an optimization solver for convex optimization problems and a heuristic for optimization problems with non-convex functions. It is built on JuMP and MathOptInterface in Julia, and solves Mixed-Integer Non-Linear Programs (MINLPs) efficiently. The solver has been peer reviewed and presented in [29].

Alpine[12] – glob(**Al**) o(**p**)timization for mixed-(**i**)nteger programs with (**n**)onlinear (**e**)qua-tions – is a novel, Los Alamos developed global optimization solver. It is built upon JuMP and MathOptInterface in Julia, and uses an adaptive, piecewise convexification scheme and constraint programming methods to solve non-convex Mixed-Integer Non-Linear Programs (MINLPs) efficiently. MINLPs are typically "hard" optimization problems that appear in numerous energy systems applications, of which Alpine globally solves by: analyzing the problem's expressions (objective and constraints) and applies appropriate convex relaxations and polyhedral outer-approximations; and performing sequential optimization-based bound tightening and an iterative adaptive partitioning scheme to piece-wise polyhedral relaxations with a guarantee of global convergence. The solver has been peer-reviewed in a variety of venues, for example [30], [31].

MINLPLib[13] is an large collection of Mixed-Integer and Continuous Nonlinear Program (MINLP) instances. These are useful for benchmarking Julia-based MINLP solvers – such as **Juniper** and **Alpine** – by performing rigorous numerical experiments, and for viewing meta information of each instance to assist analyses and experiments.

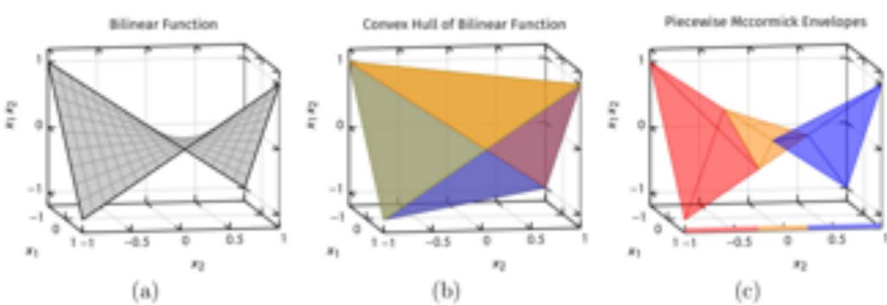


Figure A-1: The cross-sections of a bilinear term with adaptive partitioning.

[11] https://github.com/lanl-ansi/Juniper.jl
[12] https://github.com/lanl-ansi/Alpine.jl
[13] https://github.com/lanl-ansi/MINLPLib.jl

Appendix A: Developed Computational Solvers

RestartSQP[14] – Restart (S)equential (Q)uadratic (**P**)rogramming – is a solver for constrained nonlinear optimization based on outer approximation technique and is a new start effort funded by Los Alamos LDRD.

Gravity[15] is a modeling language for mathematical optimization and machine learning, which is at the heart of first-place team for ARPA-E's Grid Optimization competition and winner of the 2021 COIN-OR cup[16].

[14] https://github.com/lanl-ansi/RestartSQP
[15] https://www.gravityopt.com/
[16] https://www.coin-or.org/

Appendix B: InfrastructureModels Ecosystem

InfrastructureModels is an integrated open-source software ecosystem for modeling critical infrastructure networks. The core packages of this ecosystem – for independent, interdependent, and interconnected energy infrastructures – are introduced below. *This ecosystem provides a complimentary co-optimization capability to the DOE's co-simulation capabilities like HELICS.*

PowerModels[17] is a Julia/JuMP package for electrical power transmission network modeling and optimization. It is designed to enable the computational evaluation of emerging power network physics formulations and algorithms in a common platform. The code is engineered to decouple problem specifications (e.g., optimal power flow, optimal transmission switching, transmission network expansion planning) from the power network formulations (e.g., AC, DC-approximation, SOC-relaxation). This enables the definition of a wide variety of power network formulations and their comparison and validation on common problem specifications. The modeling approaches have been peer reviewed in [12].

Figure B-1: Brand used for the PowerModels software.

GasModels[18] is a Julia/JuMP package for natural gas transport network modeling and optimization. It is designed to enable the computational evaluation of natural gas network formulations and algorithms in a common platform. The code is engineered to decouple problem specifications (e.g., optimal gas flow, expansion planning, load shedding) from gas network formulations (e.g., steady-state, transient, approximations). This enables the definition of a wide variety of gas network formulations and their comparison and validation on common problem specifications. The modeling approaches have been peer reviewed in [21], [32].

Figure B-2: Brand used for the GasModels software.

[17] `https://github.com/lanl-ansi/PowerModels.jl`
[18] `https://github.com/lanl-ansi/GasModels.jl`

Appendix B: InfrastructureModels Ecosystem

PetroleumModels[19] is a Julia/JuMP package for petroleum transport network modeling and optimization. It is designed to optimize the operations of single liquid commodity pipeline systems subject to physical flow and pump engineering constraints. The code is engineered to decouple problem specifications (e.g., optimal petro flow) from the network formulations (e.g., LP-approximation). This enables the definition of a wide variety of liquid network formulations and their comparison and validation on common problem specifications. The modeling approaches have been peer reviewed in [33].

Figure B-3: Brand used for the PetroleumModels software.

PowerModelsDistribution[20] is a Julia/JuMP package for electrical power distribution network modeling and optimization. It is designed to enable the computational evaluation of emerging power network formulations and algorithms in a common platform. The code is engineered to decouple problem specifications (e.g., optimal power flow, continuous load shedding, minimum load delta) from the power network formulations (e.g., AC, linear-approximation, SOC-relaxation). This enables the definition of a wide variety of power network formulations and their comparison and validation on common problem specifications. The modeling approaches have been peer reviewed in [34].

Figure B-4: Brand used for the PowerModelsDistribution software.

WaterModels[21] is a Julia/JuMP package for water distribution network modeling and optimization. It is designed to enable the computational evaluation of historical and emerging water network formulations and algorithms using a common platform. The code is engineered to decouple problem specifications (e.g., optimal water flow, network design) from network optimization formulations (e.g., mixed-integer linear, mixed-integer nonlinear, linear-approximation). This enables the definition of a wide variety of optimization formulations and their comparison and validation on common problem specifications. It is primarily used to build better understandings of the interdependencies between electric power and water (e.g., pump operations). The modeling approaches have been peer reviewed in [35].

Figure B-5: Brand used for the WaterModels software.

[19] `https://github.com/lanl-ansi/PetroleumModels.jl`
[20] `https://github.com/lanl-ansi/PowerModelsDistribution.jl`
[21] `https://github.com/lanl-ansi/WaterModels.jl`

CarbonModels[22] (*to be released*) is a nascent Julia/JuMP package for carbon dioxide (CO_2) transport network modeling and optimization. It is designed to enable the computational evaluation of CO_2 transport formulations and algorithms in a common platform. It includes unique features to model the different possible phases of CO_2 transport (liquid, gas, or super critical), and model operations to prevent CO_2 phase changes that can damage equipment during transport.

PowerModelsITD[23] is a Julia/JuMP package – an extension of PowerModels and PowerModels-Distribution – for steady-state integrated power transmission-distribution network optimization. It is designed to enable the computational evaluation of emerging power network formulations and algorithms in a common platform. The code is engineered to decouple problem specifications (e.g., power flow, optimal power flow) from the power network formulations (e.g., AC, linear-approximation, SOC-relaxation) on both transmission and distribution networks. This enables the definition of a wide variety of power network formulations and their comparison and validation on common problem specifications.

GasPowerModels[24] is a Julia/JuMP package for the joint optimization of steady-state natural gas transport and electrical power transmission networks. It provides utilities for modeling problems that combine elements of natural gas and electric power systems. It is designed to enable the computational evaluation of historical and emerging gas-power network optimization formulations and algorithms using a common platform. The code is engineered to decouple problem specifications (e.g., gas-power flow, maximum load delivery, network expansion planning) from network formulations (e.g., mixed-integer convex, mixed-integer nonconvex). This enables the definition of a wide variety of optimization formulations and their comparison and validation on common problem specifications [36].

PowerWaterModels[25] is a Julia/JuMP package for joint optimization of electrical power distribution and water distribution networks. It provides utilities for modeling problems that combine elements of electric power and water systems. The code is engineered to decouple problem specifications (e.g., power-water flow, optimal power-water flow, network expansion planning) from network formulations. This enables the definition of a wide variety of optimization formulations and their comparison and validation on common problem specifications.

[22] `https://github.com/lanl-ansi/CarbonModels.jl`
[23] `https://github.com/lanl-ansi/PowerModelsITD.jl`
[24] `https://github.com/lanl-ansi/GasPowerModels.jl`
[25] `https://github.com/lanl-ansi/PowerWaterModels.jl`

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