Research Statement: Scalable Decision-Making for Decarbonized Energy Systems

Society is confronting the unprecedented challenge of *decarbonizing energy systems* to mitigate climate change. To decarbonize the U.S. energy systems by 2050, we will need to produce at least 40% of the nation's total energy demand from wind and solar, which is far higher than the current 12% [24]. Achieving this goal will require extensive research efforts on decision-making frameworks to design, plan, and operate decarbonized energy systems with high efficiency and reliability. These decision problems are challenging for two reasons: (i) the unprecedented degree of uncertainties associated with renewable generations (short term) and technological advances (long term) and (ii) the increasingly complex, multiscale, and heterogeneous nature of energy networks. At the same time, the increased degree of controllability, brought by distributed energy storage and controllable loads, will dramatically improve the flexibility of the overall system and, in turn, provide the opportunity to make our energy systems more resilient against disruptions, such as extreme weather events (e.g., 2021 Texas power crisis) and societal/geopolitical issues (e.g., the global natural gas shortage caused by the Russian invasion of Ukraine). Therefore, harnessing increased flexibility while systematically dealing with uncertainties and network complexities is the grand challenge of decarbonization.

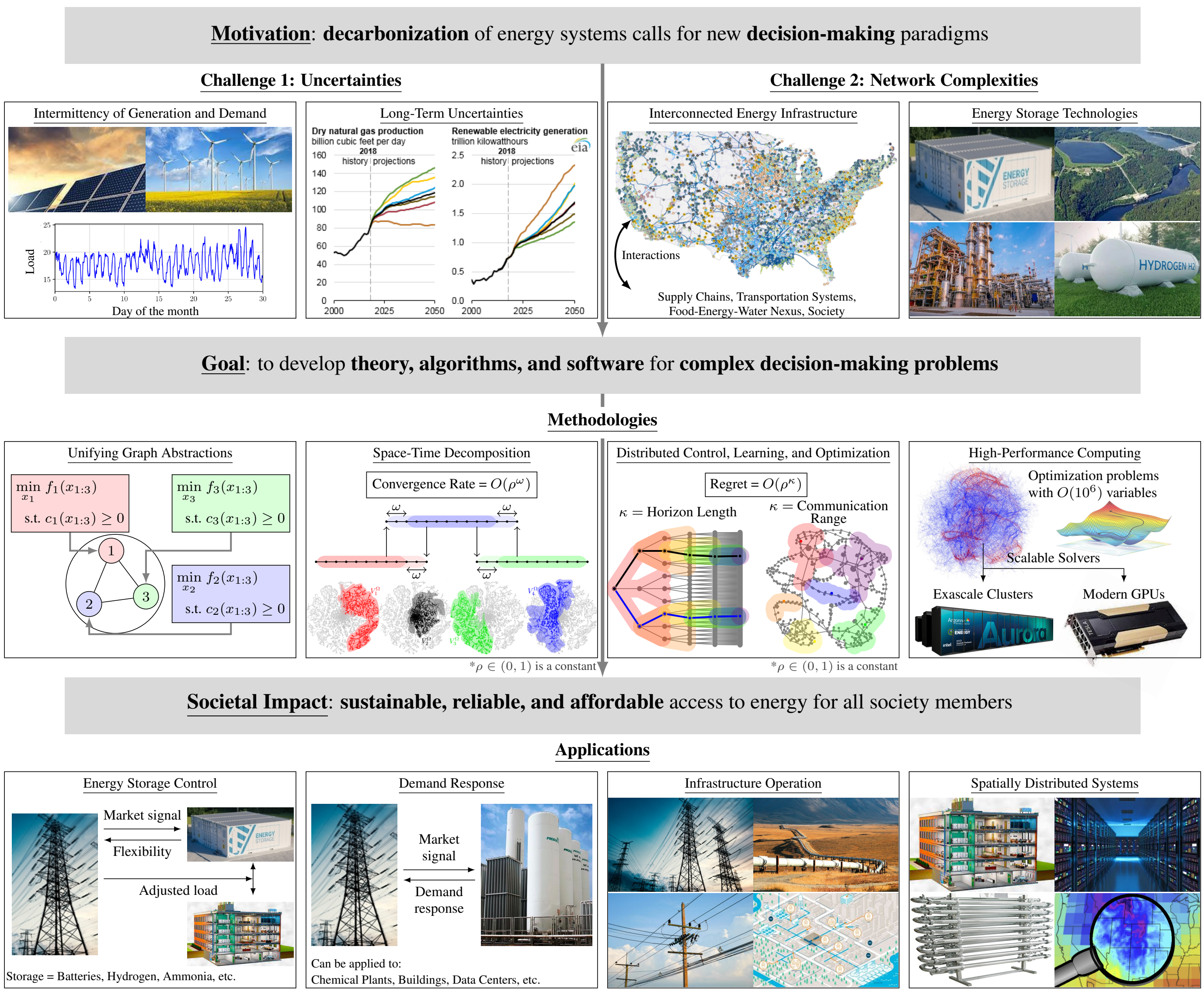

Figure 1: Overview of research interests.

My research (summarized in Figure 1) addresses this challenge by advancing the state of the art in theory, algorithms, and software implementations for complex decision-making problems in energy systems, such as sequential decision-making under uncertainty and optimization and control of networked systems. Key accomplishments of my past research are highlighted as follows. (i) Our diffusing-horizon model predictive control (MPC) strategy, applied to a heating, ventilation, and air conditioning plant, has enabled a 99% reduction in the computation time while increasing the operation cost by only 3%; with the same computational budget, the state-of-the-art reduction method incurs a 350% increase in the operation cost [43]. (ii) Our overlapping decomposition method for networked systems has enabled us to speed up the distributed solution of power system state estimation problems by a factor of 10 [44]. (iii) Our nonlinear optimization solver `MadNLP.jl` allows for solving optimal power flow (OPF) [30] and MPC problems [17] 3–10 times faster by harnessing the power of GPUs. These accomplishments have been recognized by several major awards: AICHE CAST Directors' Student Presentation Award and Young Author Awards at the IFAC International Symposium on Advanced Control of Chemical Processes and IFAC Conference on Nonlinear Model Predictive Control.

My future research will focus on addressing the unprecedented computational challenges brought by the ambitious decarbonization goals. I will study the theory and algorithms for (i) stochastic sequential decision problems and (ii) network optimization problems that can have an impact on real-world applications, such as energy storage control, operation of electrified manufacturing facilities, critical infrastructures (power transmission/distribution systems and natural/hydrogen gas networks), and spatially distributed systems (building HVAC systems, data centers, and climate systems). Furthermore, I (with the open-source coummunity) will build a software ecosystem for modeling/solution of energy system optimization problems, whereby our research outcomes can be made accessible to a wide audience in the academia, industry, and government. These efforts will provide technological advances for decarbonization, with the ultimate goal of enabling sustainable, reliable, and affordable access to energy. The proposed research encompasses conceptual and applied work that can attract funding from NSF (e.g., CBET [1, 2], ECCS [3], CMMI [4, 5], DMS [6]), DOE (e.g., Early Career Program [7] and Office of Science: ASCR [8] and HPC [9]), and industry. My connection with DOE national laboratories (Argonne and Los Alamos) will be leveraged to collaborate with their scientists and have access to their world-class computing facilities.

The remainder of this document is organized as follows. Section 1 describes the specific research activities that I have undertaken to tackle the grand challenge of decarbonization. Section 2 describes the detailed outline of the planned future research on (i) sequential decision-making under uncertainties, (ii) network optimization, and (iii) software implementation for energy systems. For each future research project, potential funding sources are listed.

1 Past and Current Research

Unifying Graph Abstractions. The operation of energy systems requires solving large-scale, but structured, optimization problems. For example, the production planning problems for power grids are formulated as long-horizon dynamic optimization; the energy arbitrage problems for battery systems take the form of optimization over scenario trees; the gas network operation problems are partial differential equation (PDE)-constrained optimization; the OPF problems are formulated as optimization problems over networks. Structures such as time horizons, scenario trees, discretization meshes, and networks can be expressed in terms of graphs; this capability has motivated us to study a unifying graph abstraction of optimization problems, coined graph-structured optimization problems (Figure 2)[35]. Using this abstraction, in collaboration with *Prof. Mihai Anitescu* (Argonne National Laboratory & University of Chicago), *Prof. Timm Faulwasser* (TU Dortmund University), and *Prof. Mario Zanon* (IMT Lucca)I have established a fundamental property that we call *exponential decay of sensitivity* (EDS) [44, 38, 37](Figure 2). Building on the classical theory [33], we have shown that the solution sensitivity against parametric perturbation decays exponentially with respect to the distance from the perturbation point under standard regularity assumptions. This result is significant in that exploiting this property allows for the creation of scalable algorithms for graph-structured optimization problems [44, 43, 29, 39, 40].

Overlapping Schwarz: A New Decomposition Paradigm for Large-Scale Optimization. Energy infrastructure optimization problems may contain millions of variables and constraints because they often embed complex networks,

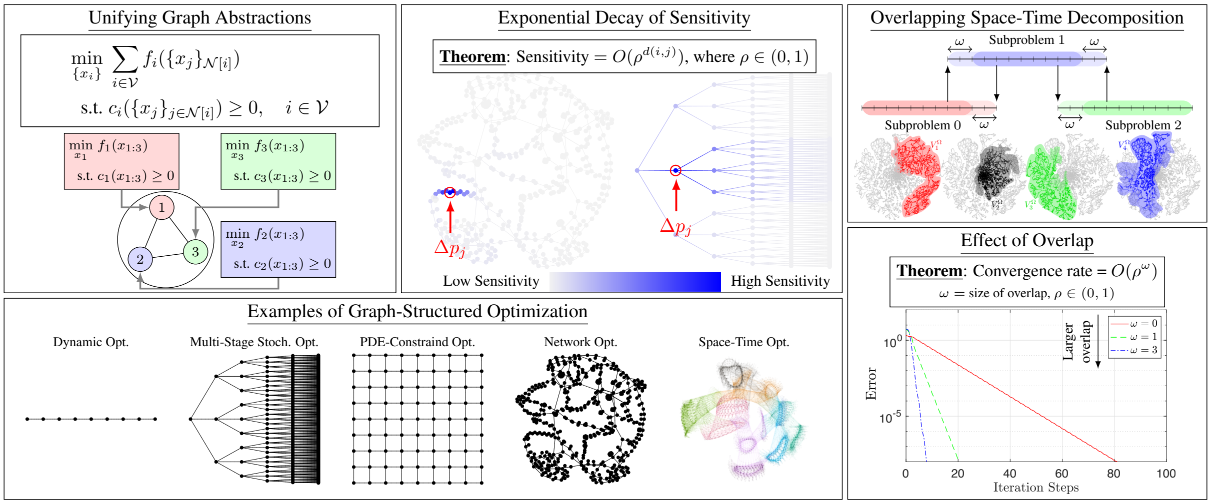

Figure 2: Unifying graph abstraction and its applications to scalable optimization.

PDEs, and uncertainty scenario trees; for example, the stochastic gas network operation problem studied in our recent work contains 1.7 million variables and constraints [18]. These problems defy the scope of off-the-shelf optimization solvers and call for scalable, distributed solution algorithms. We have developed a distributed optimization algorithm that we call the *overlapping Schwarz method*, which exploits the EDS to enable a scalable solution (Figure 2). The key idea behind the algorithm is to decompose the original problem into subproblems over overlapping subdomains and solve them in parallel and iteratively with the exchange of solution information. The method is named after the Schwarz preconditioning method [13]—a widely used algorithm for PDEs—because this method can be interpreted as a generalization of the original Schwarz method. Based on the EDS, we have shown in a number of different settings that overlap exponentially accelerates the convergence of the overlapping Schwarz method [44, 38, 29, 36]. With this method we can solve power system state estimation and optimal control problems an order of magnitude faster than state-of-the-art decomposition methods [44, 29] and solve multiperiod OPF and gas network operation problems with millions of variables [35]. This algorithm can harness the power of parallel computing clusters, such as *exascale* machines [10], as demonstrated in [44]. These capabilities have been made easily accessible through our software implementations: (1) MadNLP.jl, a nonlinear optimization solver, developed with Dr. Carleton Coffrin and Dr. Kaarthik Sundar at Los Alamos and Dr. Francois Pacaud at Argonne, and (2) Plasmo.jl, a graph-based modeling platform, developed with members of Prof. Victor Zavala's group [35, 22, 18].

Near-Optimality Analysis: A New Frontier of Control Theory. Under the decarbonization scenarios, the energy systems are likely to be operated with a tight economic margin. For example, a recent study suggests that complete decarbonization of the U.S. energy systems by 2050 would raise total costs by 69% [24]. To convince the general public that such significant decarbonization is a viable path forward, the scientific community must demonstrate that the energy systems can be operated at *near-optimal economic efficiency in a reliable manner*. Clearly needed, then, is development of *scalable control methods* with *provable near-optimality guarantees*. Achieving this dual goal is challenging, however, since often one must make a trade-off between performance and computation cost. In this context, the EDS provides a theoretical basis for designing scalable and near-optimal control policies. In my Ph.D. research, I demonstrated that exploiting the EDS in a central HVAC plant operation allows reducing the computation time by a factor of 100 while reducing the operation cost by 3%; with the same computational budget, the state-of-the-art method incurs a 350% increase in the operation cost [43].

In my postdoctoral research, I moved a step forward and established rigorous end-to-end performance guarantees for two well-known control strategies—distributed control and stochastic MPC (Figure 3)—in collaboration with Prof. Adam Wierman (Caltech), Prof. Guannan Qu (Carnegie Mellon University), and Dr. Sen Na (UC-Berkeley). Distributed control employs a set of local controllers that make control decisions using local information within a prescribed communication range. Stochastic MPC makes control decisions by planning out the decisions over a truncated scenario

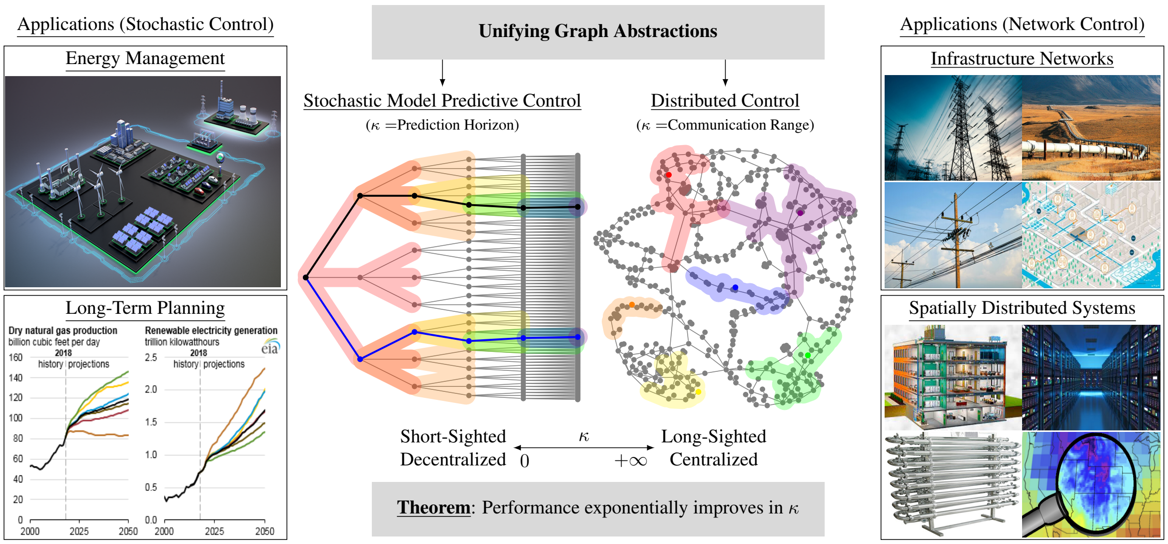

Figure 3: Near-optimality of stochastic model predictive control and distributed control and their applications ares.

tree. Building on the EDS, we have proved that these controllers can achieve near-optimal closed-loop performances under suitable regularity assumptions [39, 40]. That is, we can tune one of the controller parameters (specifically, the communication range of distributed control and the scenario tree length of stochastic MPC) in such a way that the optimality gap becomes arbitrarily small. For example, with power system frequency control, we have demonstrated that distributed control can reduce the optimality gap by a factor of 100 by expanding the communication range only by 1 [39]. Furthermore, our results answer the long-standing question of the price of decentralization in distributed control and the price of truncation in MPC [27, 28]. Moreover, our performance analysis technique improves the conventional performance analysis approaches [45, 21] in that our method can provide *a guiding principle for trading off performance for scalability* by expressing the optimality gap in terms of the key design parameters.

2 Future Research Plans

My future research aims to advance the state-of-the-art in three thrusts: (i) sequential decision-making under uncertainty, (ii) optimization of networked systems, and (iii) software implementations for modeling and optimization. Furthermore, I will aim to develop algorithms and software tools that can be deployed in real-world applications such as energy storage systems, electrified chemical manufacturing facilities, and energy infrastructures.

2.1 Optimization and Learning for Sequential Decision-Making under Uncertainty

Under the decarbonization scenarios, energy systems must be operated in an uncertain and time-varying environment (Figure 4). Therefore, to plan and operate decarbonized energy systems with high degree of efficiency and reliability, one must rigorously take future uncertainties into account while taking advantage of the ability to make recourse decisions. However, rigorously accounting for the uncertainties is challenging. For example, the intermittency of renewable generation introduces frequent supply-demand imbalances that, in turn, cause volatility in the electricity price; as can be seen in the CAISO market data [34], the real-time electricity price may jump from -$200/MWh to $300/MWh in just ten minutes. Such a high variability in the electricity price makes it challenging to economically operate electrified manufacturing systems and to build energy management systems [19]. Also, the future renewable generation capacity is subject to substantial long-term uncertainties; for instance, the 95% confidence interval for the estimate of solar generation costs in 2050 ranges from $2 to $40 per MWh [47]. This requires the long-term planning of energy systems to consider multiple future scenarios as a hedge against the risks. In this context, scalable algorithms and computing strategies are needed to deal with such challenging stochastic sequential decision problems.

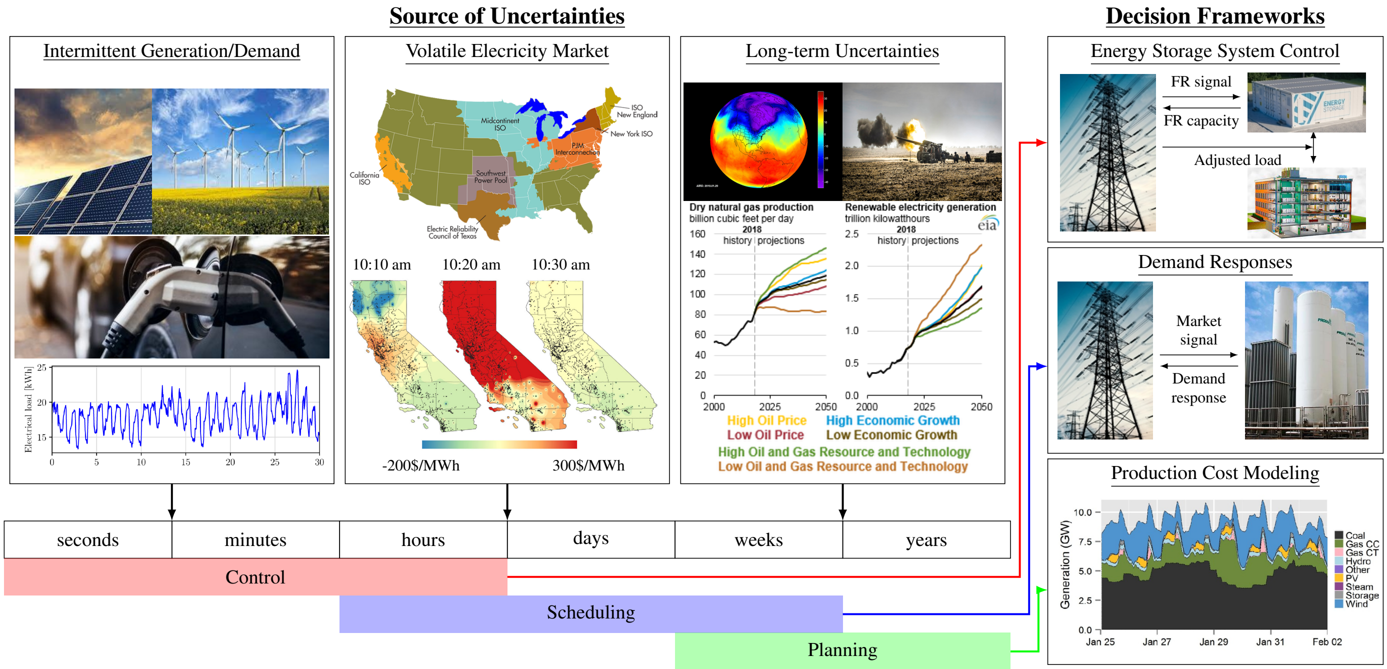

Figure 4: Uncertainties in the decarbonized energy systems and multiscale decision frameworks

Breaking the Intractability with Constrained Policy Optimization. The operation of decarbonized energy systems requires handling exogenous, nonstationary uncertainties [15]. The state-of-the-art method for such problems is the multistage stochastic programming. Unfortunately, this approach quickly becomes intractable because of the exponential explosion of the uncertainty scenario tree, and solving the problem to optimality is challenging even with state-of-the-art decomposition methods [31]. This situation motivates the investigation of an alternative approach, *direct policy optimization* with *state augmentation* (proof-of-concept presented in [41]). In this method, the nonstationary stochastic process is embedded in an enlarged Markov decision process through the state augmentation technique [12], and the problem is recast over policy parameter space. To ensure the Markov property, one needs to incorporate all the information that is in principle adequate for forecasting future uncertainties. For instance, to accurately forecast wind/solar generation, one must incorporate spatiotemporal climate data. The state augmentation strategy has never been applied to such an extent, and accordingly the resulting policy optimization problem displays several unprecedented challenges, such as (i) the high dimensionality of the state-action space and (ii) the need for constrained neural network training. Based on my expertise in large-scale nonlinear optimization, I will investigate scalable solution algorithms for such policy optimization problems. Also, to examine the performance of the method under a *data-driven, model-free setting*, I will study the effectiveness of this approach when used in conjunction with nonlinear system identification methods and compare it with closely related methods in reinforcement learning [23]. Existing funding opportunities that can support this work include the Dynamics, Control and Systems Diagnostics program (NSF/CMMI) [4].

Near-Optimality of Closed-Loop Scheduling and Planning. Planning (e.g., production cost modeling) and scheduling (e.g., unit commitment) play essential roles in the mid- to long-term operation of energy systems [11, 26]. These problems are formulated as mixed-integer optimization problems due to the presence of integer scheduling variables, and they exhibit the multistage structure that comes from stochastic dynamics. Computational challenges arise from (i) the inherent intractability of the stochastic sequential decision problems, (ii) the long planning horizons, and (iii) the presence of integer variables. An effective strategy to address the intractability is closed-loop scheduling and planning with truncated horizons (truncation may also happen in space and uncertainty sampling). Although closed-loop methods have been much less common in scheduling and planning than in control, recent studies report their effectiveness for various scheduling problems [32]. Based on my experience in analyzing closed-loop algorithms [39, 40], I will investigate the performance of closed-loop scheduling and planning methods. The aim is to establish a provable performance guarantee for closed-loop scheduling and planning and facilitate their adoption in practice. Existing funding

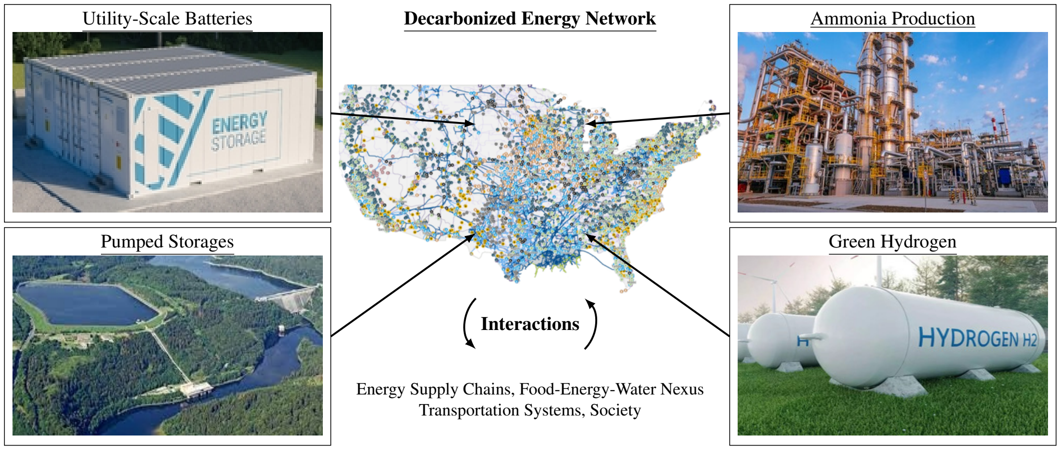

Figure 5: Interconnections and heterogeneity of decarbonized energy systems

opportunities that can support this work include the Operations Engineering program (NSF/CMMI) [5].

2.2 Optimization of Networked Systems

Efficient operation of the decarbonized energy systems will require systematic coordination of its resources; insufficient coordination can cause dangerous system failures. For example, the gas shortage during the polar vortex of 2014, partially caused by the inadequate coordination between gas and electric systems, resulted in a forced shutdown of critical power plants totaling 78 GW of generation capacity across three independent system operators (PJM, MISO, and NYISO) [25]. While centralizing the operation scheme can improve coordination, in practice it is impossible to implement centralized decision schemes because of the large, spatially distributed nature of the energy networks. Decentralizing the data and operation schemes while maintaining high performance (for any given performance metric) is challenging because of the inherent trade-off between decentralization and high performance. Building on my recent success in the graph-based approaches in decomposition algorithms and distributed control for networked systems, I will address this challenge by investigating the theory and algorithms for distributed decision-making.

Promoting Decentralization via Optimal Design. Decarbonization provides an opportunity to dramatically enhance the effectiveness of distributed operation of energy systems. In particular, our recent results suggest that distributed storage can enhance the overall controllability of networked systems and in turn, improve the performance of distributed operations [39]. However, it is nontrivial to optimally place and size the energy storage systems so that the optimal distributed performance is achieved. This situation motivates the study of formulations and algorithms for promoting decentralization. Our previous study revealed that the sensitivity decay rate becomes faster when the Karush–Kuhn–Tucker (KKT) system is well-conditioned, and the exponential decay enables more efficient decentralization [39]. Thus, the conditioning of the KKT system can be the metric of "decentralizability" and allows the formulation of optimal design problems for promoting decentralization. Technically, this problem can be cast as a mixed-integer semi-definite program, which has been studied in several different contexts [20]. I propose to further investigate the formulations and algorithms for solving such decentralization-promoting design problems. This study will provide a systematic way to harness the flexibility that decarbonized energy systems have to offer to improve the efficiency and reliability of our energy systems. Moreover, observing that the spectrum of the KKT system is related to flexibility, I will study its connection with the standard flexibility index [46]. Existing funding opportunities that can support this work include the Algorithms for Modern Power Systems program (NSF/DMS) [6].

Multiscale and Heterogeneous Networks: Properties and Algorithms. The integration of emerging energy storage technologies into the energy infrastructure is challenging because of their multiscale and heterogeneous nature (Figure 5). For example, the operation of battery systems requires considering the chemistry inside the batteries, so that the control policies do not become exploitative and degrade the long-term capacity of batteries [14]. When different types of energy storage systems are integrated into the energy infrastructure, the overall network becomes multiscale and heterogeneous because battery systems have different physical behaviors from other type of storage systems, such as green hydrogen and ammonia production facilities. At the same time, these systems simultaneously interact with other sectors such as transportation systems and supply chains (Figure 5). Therefore, the optimal operation of the overall energy system requires the coordination of multiscale and heterogeneous model components. Our existing theory—exponential decay of sensitivity [37]—does not consider such heterogeneity, and our theoretical understanding of heterogeneous networks is still limited. To overcome this limitation, I propose to study the properties and algorithms for multiscale and heterogeneous networks. This study will provide a guiding principle for the operation and design of interconnected energy systems in which a large number of heterogeneous resources at different spatiotemporal scales are integrated. Existing funding opportunities that can support this work include the Energy, Power, Control, and Networks program (NSF/ECCS) [3].

2.3 Software Ecosystem for Energy System Optimization

The computations for decarbonized energy systems require (i) flexible modeling tools for energy infrastructures and energy storage/conversion technologies, (ii) scalable optimization solvers that can handle problems with millions of variables and constraints, and (iii) a platform to connect multiple optimization models and interface them to optimization solvers. I will build a software ecosystem for such tools, which will make our research outcomes accessible to a wide audience and facilitate coordinated research on decarbonized energy systems. The blueprint of the software ecosystem I envision is described in Figure 6.

Modeling Libraries for Energy Conversion and Storage Technologies. The development of standard mathematical models and modeling libraries will facilitate computational studies of energy conversion and storage technologies. For example, the study of OPF has been greatly facilitated by the development of flexible and easy-to-use modeling libraries such as `MATPOWER` [48] and `PowerModels.jl` [16]. Motivated by the success of these libraries, several similar infrastructure modeling libraries are currently under development. One of the missing elements in the community is the modeling tools for different energy conversion and storage technologies. To address this limitation, I will lead a collaborative project that aims to develop standard mathematical models (physics-based, data-driven, or hybrid), modeling libraries, and data sets for various energy conversion/storage technologies, such as batteries, pumped storage, green hydrogen, and green ammonia. The modeling package will be particularly useful when used with `Plasmo.jl`, our graph-based modeling platform [22], since it allows us to connect the energy conversion/storage models to the gas-electric infrastructure models and solve the coupled optimization problems. The outcomes of this project will invite researchers from diverse backgrounds to study the optimization of decarbonized energy systems. Existing funding opportunities that can support this work include the Computational and Data-Enabled Science and Engineering program (NSF/CBET) [1] and Electrochemical Systems program (NSF/CBET) [2].

Numerical Optimization Solvers for High-Performance Computing. While the state-of-the-art numerical software tools are capable of solving optimization problems at a moderately large scale, they are still limited in their capability to deal with extremely large-scale problems (with millions of variables), such as those that embed scenario trees, multiscale spatiotemporal phenomena, and neural networks. In this context, recent advances in GPU hardware and the Julia language provide new opportunities for developing more efficient and versatile numerical optimization solvers. In particular, the single instruction, multiple data parallelism of GPUs can dramatically improve the efficiency of numerical software. Furthermore, the Julia language enables the development of high-performance (as fast as C) and flexible numerical software (can handle diverse data structures with a common high-level abstraction and can be even device-agnostic) at a rapid pace, as demonstrated by the recent accomplishments of the Exascale Computing Project that I was part of [10]. With these capabilities, we recently reported for the first time the competitive performance of a nonlinear optimization solver that runs on GPUs; `MadNLP.jl` running on GPUs can solve AC OPF problems 3 times faster and solve the standard linear-quadratic MPC problems 10 times faster, compared with the state-of-the-art CPU implementations [30, 17]. My research group will aim to further improve the capability of our solver `MadNLP.jl` by leveraging such high-performance computing capabilities and by implementing new algorithmic ideas. Existing funding opportunities that can support this work include programs in Advanced Scientific Computing Research (DOE/Office of

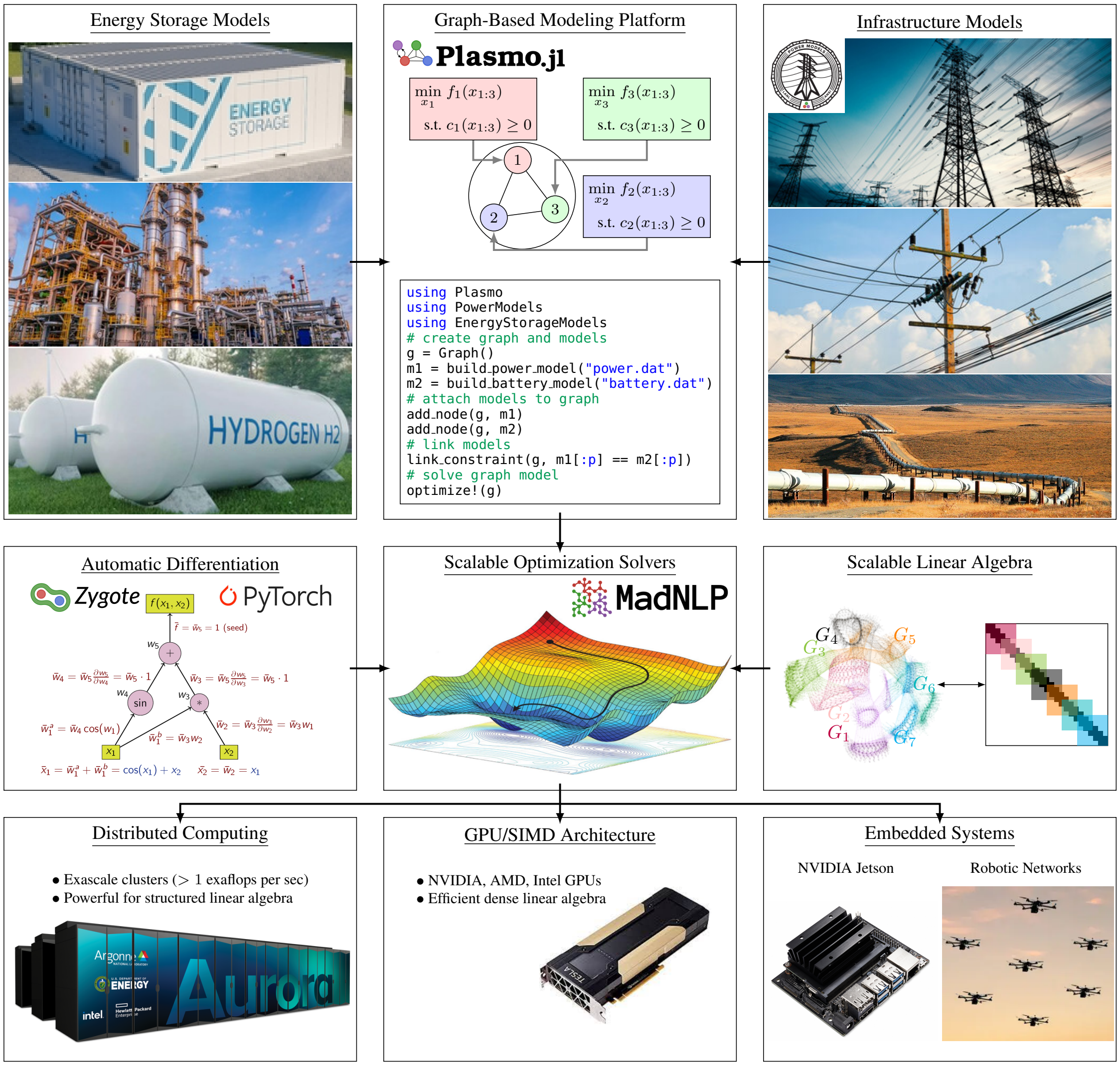

Figure 6: Portfolio of software tools and computing hardware for scalable optimization of energy systems.

Science) [8] and High Performance Computing (DOE/Office of Science) [9].

2.4 Applications beyond Energy Systems

While my past research has focused on applications in energy systems, I am eager to investigate other application areas where optimization, control, and learning can be applied. For example, during my Ph.D. studies, my colleagues and I developed a scalable parameter estimation framework for biological system models in collaboration with Prof. Ophelia Venturelli (UW-Madison). By applying our numerical solution technique based on the parallel interior-point method and automatic differentiation, we solved the parameter estimation problem in 3 minutes whereas the original approach took days to solve the problem [42]. Similarly, I will work with other research groups to discover new, challenging computational problems and use my expertise in optimization and computation to provide new insights. Furthermore, I am interested in applying our optimization techniques to problems in different application areas, such as chemical/biological engineering, environmental science, transportation science, and robotics. For example, the techno-economic analysis of new catalysts, biofuels, pharmaceutical products, and carbon capture/storage/utilization technologies can be performed in conjunction with long-term planning under uncertainty. Also, our decomposition algorithms can be useful for solving large-scale spatiotemporal inverse problems in climate systems, and the graph-based distributed control methods can be used for the control of robotic networks. I believe our optimization techniques have potential to solve many previously inconceivable problems and provide new insights.

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