Ten challenges for mathematical modeling of the energy transition

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1 Introduction

In an effort to limit global warming, the world has committed to a transition from using energy generated by fossil fuels to renewable energy. The scale of this transition is enormous, and it will be costly. A wide range of models and analytical tools have been devised to help in planning and implementing the transition. In this paper we use the term "model" to encompass analytical approaches more generally. Examples include a machine-learning approach to find good recourse actions; a computational tool that enables equilibria of markets to be found; analysis that predicts instabilities in energy systems; or a description of a policy choice under uncertainty for which an optimal solution can be found.

We will outline a set of ten significant challenges that we need to address, as a guide to where new research could be profitably pursued. Our experience convinces us that in many areas of the energy transition, we do not yet have the right mathematical models to capture important aspects of the energy transition, or the right methods to provide useful analysis. In identifying these challenges, we want to provide directions for research in this area. We have focused our attention on analytical challenges arising in the energy transition, rather than considering related technological challenges, such as carbon-capture technology or battery design.

In assessing models for the transition, we place a high value on their utility. We want the models to be realistic, understandable, and trusted, so that decision makers find them useful. Large complex models do not always satisfy these criteria. Validation on real data builds trust, but this can be difficult for long-term models, even if historical data sets enable back-testing. Ideally, models should yield new insights.

Collecting a set of challenges in one document is valuable. Doing so provides a helpful summary of the many opportunities for future research analyzing the green-energy transition. In distilling the perspectives of a number of researchers from different disciplines, this paper reflects a consensus on the most important analytical challenges in the transition.

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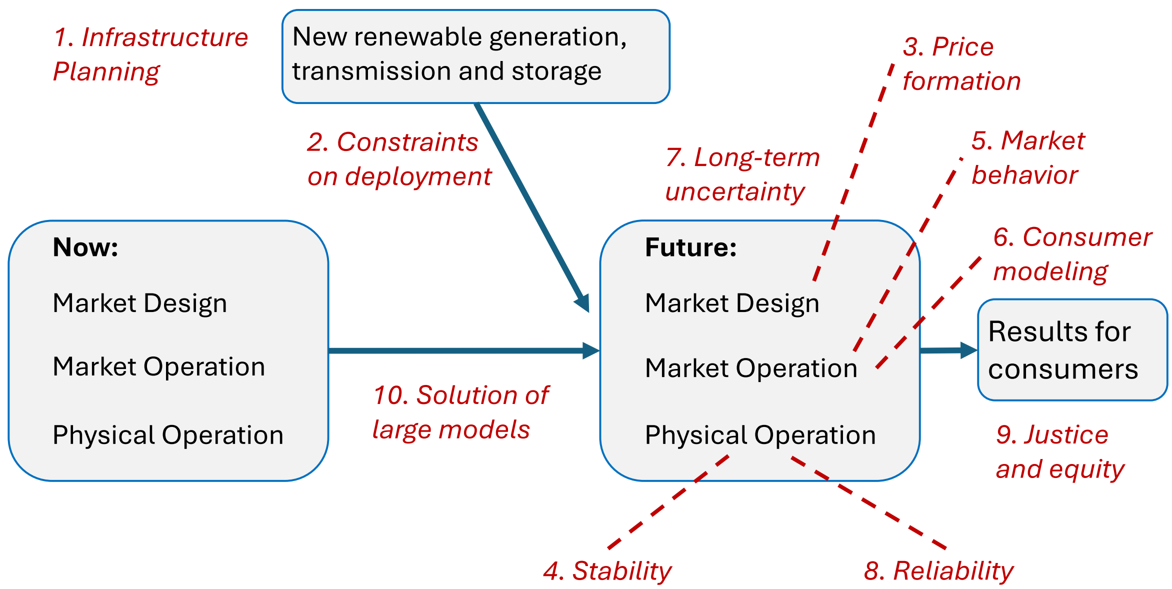

Figure 1: Overview of the challenges and where they occur within the energy transition framework.

Figure 1 shows how the ten challenges relate to the components of the energy transition. We summarize the individual challenges as follows.

We begin by considering the decisions that are needed to build infrastructure for the energy transition (Challenge 1). The green-energy transition is a matter of urgency. Thus, the transformation needs to occur at speed, which introduces constraints on the way that infrastructure is built, for which models need to account (Challenge 2). But changes in infrastructure alone are insufficient. There are also changes that are needed in the way that the electricity industry operates at both a market level, where price mechanisms may need to change (Challenge 3), and at the physical level, where mechanisms for stability and control are impacted by the switch to renewable-energy sources (Challenge 4).

Understanding the behavior of the energy system as a whole implies an understanding of how interdependent participants that interact with the system will behave. At the wholesale level, this requires the use of game theory to represent independent suppliers making strategic choices (Challenge 5) and customers' trade-offs in making energy-usage decisions (Challenge 6).

Energy systems require us to make decisions in an uncertain environment. Uncertainties occur at the macro level, when we consider investments that are made now and will be used for decades into the future in an environment that we cannot predict accurately (Challenge 7). Uncertainties occur also at the micro-level, impacting our goal to build systems that are robust to uncertain extreme events of various kinds (Challenge 8).

With large changes in the energy system, there is potential for injustice and inequity, for which one must account alongside other considerations (Challenge 9). Finally, we need to recognize that modeling the transition in an energy system which is large and complex brings its own challenges in the scale and complexity of the models built and their validation and use (Challenge 10).

In some cases, we have good versions of the models that we need but fall short of being able to analyze them, or compute solutions. In other instances, the structure of the model may be clear, but we do not have the data that we need. In other cases, we do not yet know the best way to model the problem that we are interested to study.

2 The ten challenges

Challenge 1: Policy choices for infrastructure planning.

The policy mechanisms that support major infrastructure investments need to incentivize good long-term capacity decisions, recognizing the significant uncertainty regarding what will happen during the lifetime of the assets (*e.g.*, 10 or 20 years). Costs are likely to change substantially, there is inherent policy uncertainty and volatility, and consumer demand is difficult to forecast, *e.g.*, owing to the rate of electrification (see Challenge 7).

Infrastructure-investment decisions involve interactions between many different actors, including government at various levels, market operators, transmission-network owners, and individual investors. Each of these entities make decisions within a specific regulatory and market environment, with complex connections between different decisions. A simple model of the way that this occurs may involve government determining the aggregate amount of new generation to be procured, which is followed by an auction to determine the exact mix of generation and energy storage that is built and decisions made by transmission owners regarding reinforcement of the transmission network.

Infrastructure decisions are not made once but repeatedly. For instance, generation investments are made throughout the time horizon of a planning model, and transmission capacity can be built in a reactive fashion (as generation investments are undertaken) or proactively (depending upon where generation investments are anticipated) [51, 54]. As the penetration of variable renewable energy increases, the value of dispatchable resources, including energy storage, increases. Thus, the timing of investment decisions is critically important.

In determining the appropriate level of transmission or energy-storage investment, there is a trade-off between generator curtailment when local net demand is negative, and the higher investment costs of greater transmission capacity or more energy storage [53]. An optimal capacity decision depends also on the variation of generation supply and electricity demand and details of the market design that provides price signals.

Contracting for procurement of generation capacity can take many different forms. Examples include contracts for differences, payments for curtailment, and availability payments and penalties. In addition, implementation details, *e.g.*, the length of the contract term, must be determined.

The choice of objective function for planning models is not straightforward. Due to misaligned incentives, a good outcome for one agent may not be so for another. Moreover, the relationship between outcomes may be complex. As an example, a transmission planner that preserves real options, *e.g.*, by delaying investment until demand grows, might increase risk for generation capacity planners and produce an outcome that reduces social welfare.

Infrastructure-planning models give different results depending on the order in which decisions are made and when information becomes available, and this may be difficult to determine. For example, it is unclear whether transmission-investment decisions lead generation-investment decisions or vice versa. Regardless, the sequential and autonomous nature of these decisions can create investment dynamics, signaling games, and information asymmetries that can yield socially undesirable outcomes.

Challenge 2: Constraints on deployment.

The urgency of decarbonization implies that changes to the energy system need to occur very rapidly, with a massive deployment of renewable generation and other sustainable technologies. The need to move fast leads to bottlenecks and supply-chain problems.

Given the constraints on the availability of various resources, the timing of our deployment actions becomes important. We need models that reflect these constraints to answer questions regarding what is feasible, what should be given priority, and what are low-regret actions that should be taken first.

The resource constraints relate primarily to the supply chain. Ramping-up wind-turbine production is only possible if there are sufficient manufacturing capacity, raw materials, and the requisite logistics to transport and install the massive required equipment. For photovoltaic solar, there are shortages of key materials [38].

There are also questions about the scale of the manufacturing enterprise that is required and the energy consumption that is implied by the manufacture of energy storage or wind turbines. Building renewable generation involves the use of energy that is associated with carbon emissions [16]. Different policies for the sequence and the speed of manufacture of the products that are needed for the energy transition will give different results in terms of total emissions. The problem of finding the right trajectory here is reminiscent of the classical bottleneck problem that is formulated by Bellman [4]. Modeling this problem could involve examining the implications of learning effects (see Challenge 7).

Often, there are constraints that arise from a shortage of appropriately skilled workers. These are seen acutely in large-scale roll-outs of new technologies at the consumer level. An example occurs in the shortage of heat-pump engineers to conduct home installations. More generally, there is a global shortage of electrical engineers and other skilled workers that are needed for the green-energy transition [33].

Another form of constraint might be called "planning overload". This is seen most clearly in the ballooning of (inter-)connection queues around the world [34]. The queues consist of new renewable-generation projects that are waiting to be connected to electricity systems. Each such (inter-)connection requires an impact study to understand the requirements for electricity-system strengthening and without sufficient resources to fast-track all of these, queues grow longer and longer. There is a related difficulty in going through the necessary processes to obtain planning permissions for new renewable generation and the increased transmission that is also needed. In many countries these constraints are sufficiently severe that they can rule out reaching some of the short-term intermediate emissions targets that are proposed.

Models that respect capacity constraints over time may have different characteristics depending on the time horizon involved. Relatively short-term problems, such as occur in (inter-)connection queues, need to consider a scheduling perspective, so that the sequence in which actions are conducted becomes important. Longer-term problems are likely to involve considerations of optionality. Decisions on what is done first have an impact on future decisions, which depend on what has happened so far (*e.g.*, in the price of key materials).

Challenge 3: Price formation in wholesale markets.

Wholesale electricity markets use price as a means to guide behavior. Price formation is essential to support efficient decision making. If the prices are wrong, the decisions (*e.g.*, production, consumption and investment) will be wrong. Inefficient prices can arise from non-convexities, the exercise of market-power, or missing or illiquid markets for risk products.

Existing wholesale markets can come close to the ideal of prices reflecting marginal social utility. The US day-ahead and real-time markets send time and location signals that induce highly efficient dispatch and scheduling of traditional supply resources [14]. However, today's markets fall short of accommodating energy-storage and demand-side resources. When wind and solar penetrations are high, wholesale electricity prices will become volatile if demand is inelastic, swinging between zero (or even negative values [52]) and the value of lost load. Dispatch and pricing mechanisms that correctly incentivize participation of demand-side bidding and energy storage are needed.

Many research questions emerge from efforts to improve market rules. For example, current models for price formation are multi-period economic-dispatch models, that are solved in a rolling-horizon fashion. These models deal with non-convexities from unit commitment through various forms of convex-hull pricing. Even in the convex case, dispatch and prices can be inconsistent with agents' preferences when viewed *ex post*.

At shorter time horizons, real-time dispatch models can be improved with some form of look-ahead that recognizes resource constraints or future opportunities that arise during short periods. When the future is uncertain, flexibility has a value that should be rewarded and using stochastic dispatch models is one approach to such valuation. However, agents must agree on this stochastic model and, as with multi-period models, they may not yield time-consistent dispatch and prices. Spot markets, day-ahead to real-time, enable efficient operation of existing resources. Longer-term price signals are needed to motivate investment and let participants establish positions to manage needs and risks. Forward markets play a crucial role in enhancing the efficiency and stability of electricity markets by addressing issues such as risk, market power, and investment coordination [15]. Liquid forward markets enable price risks to be hedged and reduce volatility in the cash flows that are needed to support investment. By allowing new entrants to compete before entering the market, forward markets foster competition and reduce uncertainty. Moreover, by shifting a significant portion of trading from spot markets to forward contracts, forward markets reduce the incentive for suppliers to exercise market power during periods of scarcity.

Models are needed to inform the design of forward markets. These markets must maintain liquidity across many interrelated products and have sufficient spatio-temporal granularity to be (close to) complete. Risk-management tools are needed also for suppliers and load-serving entities, including retail rate plans that maximize value for consumers while limiting risk [5].

Challenge 4: Stability and control of systems with high renewables.

The rapid increase in green energy is prompting concerns about increased variability in electricity systems at multiple time scales and how to control such variability. This variability represents three challenges:

1. Wind and solar renewable resources are intermittent, which requires supplemental energy supply;
2. Retiring conventional plants reduces system inertia; and
3. Inverter-based resources can introduce new forms of electricity-system instability across multiple time scales.

Much has been written about the costs of integrating variable renewable energy (like wind and solar) into existing high-voltage transmission systems [30]. When the wind does not blow or when the sun goes down, backup generation is required. This backup supply comes from various technologies (*e.g.*, energy storage or peaking generation) that are dispatched by a balancing market, or such resources are aggregated with wind or solar so that a firm supply can be offered to the market. Dispatching backup generation through the grid is more efficient, but requires multi-period dispatch models that are solved in a rolling-horizon fashion using forecasts. During 2023, CAISO used a 65-minute horizon with five-minute increments to compute locational marginal prices [44]. This market design can lead to pricing inconsistencies, which increases uplift payments [11].

Conventional generators produce electricity from heavy rotors that spin at a nominal frequency. The angular momentum due to the inertia of these spinning devices serves to dampen fluctuations in frequency from random events. In most markets stability requirements are typically met by ancillary services (although security-constrained dispatch in some markets procures reserve from market offers). As the cost of providing stability services grows with the growth of variable renewable generation, the services can be included in a market settlement (as spinning reserve is in some markets). This is a challenge that will become more pressing as distributed renewable energy resources are aggregated into virtual power plants [31]. Renewable generation is converted to AC using power electronics [41]. The dynamic behavior of power electronic converters is dominated by the enforced control law [25]. If inverters are set to match the observed frequency, then fluctuations in the latter can cause inverters to follow a dropping frequency with risk of system collapse. For example, during the 2021 Odessa event [13], a fault at a Texas combined-cycle generator resulted in power reduction for solar plants totaling 1 GW of capacity (a quarter of those operating at the time). This power reduction was not due to the fault itself, but due to inverter-level or feeder-level tripping or control-system behavior within the resources.

New developments in so-called grid-forming inverters endow these devices with software that responds to system disturbances more intelligently [35]. Grid-forming inverters have been deployed successfully in small-scale systems. Although the small-disturbance behavior of inverter-based systems can be made to match synchronous-generator dynamics, their large-disturbance behavior displays hybrid dynamics due to inherent limit-induced events [32], which is quite different from synchronous generators. Rather than performing case-by-case analyses, the challenge is to build general models for understanding the behavior of heterogeneous types of inverters in large systems that are susceptible to large disturbances.

Challenge 5: Predicting the behavior of wholesale energy market participants.

Wholesale energy markets are becoming more complex as a result of the energy transition. There are a greater number and variety of generation participants including an increased role for non-dispatchable generators; an increased amount of demand-side response; a greater geographical spread of generation (including imports from different countries); and increased short-term uncertainty in supply. Existing ancillary services, such as reserve and fast-acting response, will become more important, alongside new services, such as the provision of inertia (Challenge 4). Predicting the behavior of market participants has become harder.

The decarbonization imperative makes it important to model how energy-market participants respond to incentives. Real markets will have imperfections. We should use models to understand and avoid the impacts of these imperfections. In studying wholesale markets, we typically assume rational agents who will make decisions to maximize profits (or utility). We then assume that market participants follow an equilibrium strategy, which is computed using the best model of these profits that we have available.

Equilibrium behavior for wholesale-market participants involves bids and offers that may take different forms depending on the jurisdiction. Trade can occur during different times, with forward contracting, day-ahead auctions, the possibility of during-the-day adjustments, and a market to balance generation (as well as demand) during real time. Different participants will have different information.

Any proposed market design should maximize welfare in the setting of perfect competition and complete markets [21] as a minimal requirement. In reality, large generators often will be aware that they have market power to affect prices [27], while facing risks that cannot be hedged [1].

The starting point for comparison is the full-information (Nash-)equilibrium set of bids and offers. But this can be difficult to find: there may be no equilibrium in pure strategies and there may be multiple possible equilibria (*e.g.*, in many supply-function models there is a continuum of equilibria). To enable predictions in real situations these models typically have to be large scale, which poses a computational challenge. Finding one equilibrium may not be enough, and there are no current effective methods for computing all possible equilibria.

There is a tension between the relative simplicity in, *e.g.*, cost structures of many game theoretic models and the complexity of electricity systems. As the number of empirically important markets grows, generators need to consider how to allocate their capacity across multiple products, such as energy and reserve, or submit multi-part bids to the system operator to signal separate start-up and energy costs [18]. In systems with locational prices, the quantity that is offered in one place will also affect prices elsewhere, so that the best response function becomes a hyperplane [27].

Because the market operates repeatedly with the same set of participants, we can expect learning to occur, so that behaviors vary over time. Participants that react repeatedly to new circumstances might make their actions seem irrational and hard to predict. We can consider also the possibility of implicitly collusive behavior, where there is a non-competitive outcome, but market participants have no incentive to change this.

Both types of outcomes can distort market efficiency, but collusion is particularly hard to model. The "Folk Theorem" [24] implies that there will be many different possible collusive outcomes. The use of reinforcement learning in bidding processes [56] may well increase the likelihood of collusive outcomes, without this being a deliberate choice of participants.

The overall aim of modeling is to develop tools to enable better prediction of actual outcomes. However, comparing predicted with actual bids is not straightforward, since the information behind the actual decision may not be available. It is a challenge to model the information available to the different participants and their individual circumstances (*e.g.*, their beliefs about other players, the financial contracts they hold, and their risk attitudes).

Challenge 6: The impact of consumer decisions on the energy system.

Some important components of the energy transition, especially distributed photovolatic-solar production and increased electric-vehicle usage (with or without vehicle-to-grid operations) push the energy system toward more decentralized operation. In particular, more operations happen closer to the consumer, leading to a growing importance of the distribution system—and its limits—by comparison to the transmission system. For example, a transformer that currently is adequate for a residential area is short of what is required if 75% of the houses choose to charge their electric vehicles simultaneously. Thus, the design of the distribution network (*e.g.*, transformer sizes, line capacities, and topology), as well as its operation, must be optimized to accommodate these potential future requirements.

If centralized, electric-vehicle charging can be sequenced so as to limit peak consumption. However, charging is a consumer's choice that can only be incentivized, with finer control attainable through automation. It is possible also that automated charging in a way that over-responds to wholesale prices will give rise to problems with new demand peaks [36]. Therefore, one might ask what is the right way to model the householder and business decisions on the demand side (*e.g.*, vehicle charging) and the way that these decisions interact with the rest of the market through aggregators? More broadly, tools that model options at the "grid edge" (*i.e.*, the distributed hardware, software, and business innovations that exist in proximity to the end user) are needed.

Understanding consumer choices requires modeling retail markets and consumer behavior [23]. The gap between retail and wholesale markets is being closed with increasing granularity of pricing options for businesses and individual consumers. Retail-market design varies from simple time-of-use pricing to incentive-based schemes and automated demand response. At the extreme, consumers may opt for real-time pricing [28]. The use of home automation offers many possibilities for demand to respond to prices, including delegating control to a third-party in charge of satisfying the consumer's needs for an agreed upon price. It is necessary, however, to understand the barriers to implementing such mechanisms at the household level [46, 20]. The absence of demand response has long been recognized as a significant cause of inefficiencies in energy systems.

The householder has various options to reduce or to shift demand. Some of these options require appliance automation, (*e.g.*, a refrigerator that delays the start of the cooling cycle under some circumstances), others may require a decision (*e.g.*, delaying starting the washing machine or adjusting a heating schedule when anticipating being away). We require models that capture household behavior, possibly through categorizing them according to their characteristics [55]. Getting a finer comprehension of consumer behavior might require the use of data science methods [57], which raises privacy concerns [40].

Challenge 7: Dealing with long-term uncertainty and the associated risks.

The implementation of the energy transition must account for uncertainty. First, there is uncertainty about the long-term effects of climate change, *e.g.*, extreme temperatures or droughts, on energy systems. Second, electricity demand will increase in the future as the residential, transportation, and industrial sectors become more electrified, and new services emerge. The rate of this increase is hard to predict. Future costs are uncertain, not only because of unforeseen technological advances but also because of the learning process in manufacturing that typically leads to cost decreases over time. Finally, there is uncertainty about the way that regulations and government policy (*e.g.*, carbon charges) will change.

The system-optimization models that are used by policy makers and stakeholders do not represent the long-term uncertainties and associated risks faithfully. If modeled at all, uncertainties are nearly always represented using finite sample spaces, yielding a set of "scenarios" [19], each of which is a possible realization of a sequence of random events that occur independently of any actions or policies. Estimation of probabilities for scenarios in these long-term models is a challenge. Computational challenges also arise when solving multistage optimization problems where uncertainty is represented by large scenario trees, as complexity typically grows exponentially with the number of stages.

Policy makers (and many in the energy modeling community) often define "scenarios" differently: they are a possible narrative of future events and decisions under some broad assumptions about the future. These make sense when used to simulate fixed policies. A challenge is to incorporate and communicate to policy makers the notion that decisions obtained with optimization cannot depend on future information, to enhance understanding of the use and misuse of scenarios.

Optimization under uncertainty becomes more difficult when uncertain parameters are affected by decisions. Typical examples arise in optimizing the tradeoff between exploiting actions known to give satisfactory results and those that riskily explore for potentially better outcomes (as occur in bandit algorithms [37]). Optimizing subsidies for technologies (*e.g.*, solar panels) to improve learning is another example [26]. Such models can often be solved using mixed-integer programming [29], but they are limited to small-scale problems.

Investors will choose technologies that they perceive to be promising. Uncertainty over these choices will affect decisions that are made by other investors. While some of these issues are identified in the economics literature [47], much remains to be done to include such uncertainties appropriately into optimization models that are used for planning. Investors will have different risk attitudes and time-based preferences (discount rates) [39]. Models must integrate the selfish decisions of investors to maximize their own risk-adjusted welfare subject to any government policy objectives. Integrating such ideas with long-term optimization constitutes an important challenge.

Another challenge relates to model mis-specification. Here we refer not only to mis-specification of probability distributions as discussed earlier, but also mis-specification of the model itself. For instance, ignoring the dependence of the uncertainty on the decisions can have disastrous consequences; Cooper *et al.* [12] present simple models to demonstrate this effect, albeit in a different context.

Challenge 8: Reliability and resilience to extreme events.

Power-system engineers balance the risk of system failures against the cost of everyday performance. Climate change has led to an apparent increase in the frequency of once-in-a-century events, which creates a need to account more for such extreme events in planning, thereby affecting this balance.

We can distinguish different types of extreme events. Some, such as earthquakes, are unpredictable and the focus will be on the efficient physical recovery of the system to a good operating state. While the green-energy transition may lead to new options, due to a more distributed supply or movable electrical storage, existing modeling techniques can be used to find appropriate sizing, staging, and operation during this recovery.

A more significant challenge is to find the strategies we should follow in predictable extreme events, such as those that are associated with weather systems. Understanding the frequency, scale, and impact of the event is critical to address these questions. There is potential for severe consequences from such events, such as the widespread power outages caused by Winter Storm Uri in Texas during February 2021 [8]. Many events are highly correlated due to their dependence on weather, especially temperature. Storms, hurricanes, destructive wildfires, heatwaves, drought, torrential rains, and flooding can have severe impacts on both electricity supply and demand. Extreme temperatures tend both to increase power demand and to decrease power supply [42] and have contributed to major power outages and near-shortage events during recent years. Data-driven approaches that form better predictions, coupled with approaches that incorporate learning [17], are needed to optimize effectively under such settings. In both settings, it is also important that useful forensics are generated for future planning and response, to determine what could have been done better. Capacity-expansion models (Challenge 1) have a key role to play, providing redundant generation to guard against the risk, specifically adapted to systems that are impacted by high-impact, low-frequency events.

Extreme events can lead to very high prices. There are difficult questions to address regarding whether these are an appropriate part of the market functioning, or whether there should be additional caps and safeguards in place. A related set of questions are what new instruments, or forms of reserve or ancillary services, would be valuable to help counter extreme events and how these can be validated.

Sampling approaches are difficult in these rare-event settings. Various approaches exist to address sampling issues of severe tail events [50]. One approach is importance sampling, where different weights are applied to such events. Another is to split the main model from the extreme-event model, and validate rare-event outcomes using the extreme-event model [49]. Details of how to communicate key variables (such as the need to add, say, 5% more generating capacity) from one model to the other are important to improve resilience. A feedback process between these models is necessary.

Challenge 9: Justice and equity.

The green-energy transition has very significant effects on individuals, which differ according to where they live, what capital resources they may have, their family circumstances, and their lifestyle choices. For example, significant changes in employment will occur as legacy fossil-fuel industries are replaced with renewable-energy alternatives [9]. Changes of this magnitude should not be conducted without regard to equity and justice. Lack of equity can be a powerful motivator for voters (as can the perception of unfairness). Thus, there are also political consequences, that may undermine any cross-party approach to green-energy initiatives. The challenge is to design energy markets and systems that promote justice and minimize inequities, or at the very least to ensure that injustices are not created through lack of attention to these issues.

Concepts of equity and justice are multi-faceted and there are many aspects of equity which might be considered within an electricity market design [2]. The most attention has been paid to distributive justice, relating to benefits or dis-benefits that arise for different groups of people. If a minimum amount of energy (*e.g.*, for heating) is viewed as a human right, then policies that moderate the price of retail contracts should reflect this. Disconnection of customers in times of shortage should not affect the vulnerable.

Another example of distributive justice occurs in retail markets in the allocation of fixed cost, which is often absorbed into an energy charge. This means that large energy users pay a higher proportion of the fixed cost of connection. In the past, large users were typically wealthier families in larger houses, although some people, particularly the elderly, may have high consumption despite living on low incomes. The advent of rooftop solar has allowed many households with the resources to install solar panels to reduce consumption and pay a much lower share of the fixed costs. Furthermore, it is often the wealthy who are among the first to adopt green technologies (*e.g.*, solar panels and electric vehicles) and benefit from incentives that are funded by taxpayers [7, 6].

Another aspect is procedural justice, which relates to the transparency of decision-making processes and whether they represent the interests of affected parties. For example, what steps must be followed before some communities are required to host intrusive new infrastructure such as transmission lines?

Changes to the energy system will have different implications for consumers living in different regions. An example occurs in the U.S. Department of Energy's Justice40 initiative [43], where disadvantaged communities are identified from census data, with the goal that 40% of the benefits from a range of federal investments should flow to these disadvantaged communities. A related approach is described by Chapman *et al.* [10] who give an example of equity considerations in decisions on the closure of different coal-fired generation plants.

Equity considerations should be built into models from the start. Models are useful for exploring trade-offs, so if equity can be measured appropriately, one can include this in a multi-objective optimization and look for trade-offs between different objectives (*e.g.*, reducing emissions and avoiding fuel poverty) to find a Pareto frontier.

On the other hand, equity can be considered a constraint. Model outputs can be used to determine metrics that can be used to assess the equity of the resulting decisions. These could include environmental and health impacts; access to energy services and their affordability; and community engagement and participation. If the outcome is not acceptable to policymakers, then the policy being modeled should be changed (if possible). Otherwise, another intervention should be made to offset the distributional consequences that are discovered. Equity metrics also can be recorded and used to measure how outcomes for different groups change over time and between scenarios.

Challenge 10: Computation and validation for solution of large models.

Modern electricity systems are described as the world's largest machines, involving many interconnected producers and consumers. The scale of the models that are required for their planning and operation has always posed challenges in analyzing their behavior [45]. The green-energy transition has magnified these difficulties [22]. Renewable generation has increased the importance of inter-connectors between regions and across time periods, which increases the scale of the models that are developed. These models need to support policy choices that reflect decarbonization goals over longer time periods.

Challenges occur in the following three areas: collection of realistic and high-quality input data, the formulation and resolution of the model, and the validation and interpretation of the solution.

Very large models are time-consuming to build, solve, and validate. They require large data sets to run. It is important to find ways of generating representative datasets to tame the instance size, while still capturing the underlying phenomena faithfully. This is particularly important when we wish to represent uncertainty: multi-period models scale linearly with time when they are deterministic, but increase exponentially when uncertainty is taken into account. The uncertainty may relate to wind and solar output [48] as well as longer-term issues (Challenge 7). The use of very large models that are based on enormous data sets makes this a potentially interesting area for the application of machine learning.

Along with better data, better algorithms and implementations are needed to compute solutions within time frames that are appropriate for the underlying decision problem. Algorithms that can solve the largest model instances need to exploit their mathematical structure. Modeling frameworks that can provide this information to the solvers are essential in tackling larger and larger instances. Parallel computation and advances in optimization and machine-learning software will have impact here, along with the use of specialized computational hardware for solutions.

There are different types of models that relate to energy systems of the future. For instance, integrated assessment models are used to explore different pathways that meet energy and climate targets over periods of many years. These have a wider scope than our focus here, being concerned with emissions; land and resource usage; climate impacts; and technology choices (*e.g.*, in carbon capture). We need models that are more concerned with the economic impacts of different policy choices for the green-energy transition [3].

Diagnostic tools are needed to validate the solutions and test the models. This can take various forms: for example, a model might be "back-tested" on historical data to determine if its forecasts made 10 or 20 years ago have transpired. Different models of the same region can be compared: what drives any differences in model solutions to similar problems?

To support effective policy analysis, models need to represent the diversity of actors and stakeholders with potentially competing objectives. Models which effectively handle different stakeholders are necessary to develop an understanding of the complex trade-offs that are required in energy policy.

3 Conclusion

This paper presents ten modeling challenges that arise from the transition to green energy. The broad themes are infrastructure (Challenges 1–3), short-term models of electricity (Challenges 4–6), long and short-term uncertainty (Challenges 7 and 8), justice (Challenge 9) and computation (Challenge 10). Because the focus is on the energy transition, systems for electricity generation and transmission have received most emphasis, which perhaps also reflects the backgrounds of the authors. We have not discussed green fuels (*e.g.*, hydrogen) or reducing emissions from agriculture and transport, and we have hardly touched on general integrated models as these have a much broader modeling scope (dealing with emissions, land use, *etc.*) than the energy transition alone. Our hope is that the paper will provoke discussion among modelers and policy makers, and provide a starting point for applied mathematicians, engineers, and economists who are looking for research areas that will contribute to reaching net-zero-carbon targets.

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