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SIMULATION AND AI FOR CRITICAL INFRASTRUCTURE

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ABSTRACT

Simulation and artificial intelligence (AI) have played crucial roles in the design and operational optimization of critical infrastructures in modern societies. In this work we briefly review the latest development in three fields, namely the stability analysis and supply demand matching in electric power grid, and the efficient simulation in autonomous driving. We wish this tutorial may shed some light on the synergy between simulation and AI for critical infrastructure in the near future.

1 INTRODUCTION

Simulation and artificial intelligence (AI) are playing important roles in the design and operation of critical infrastructures in modern societies. In this work, we focus on two systems which are part of the critical infrastructure of a society, namely electric power grid and autonomous driving. In particular, we will consider the stability analysis and supply demand matching in electric power grid, and efficient simulation of control policies in autonomous driving, and discuss how various simulation and AI tools are used separately or jointly in these examples. Through these three examples, we hope to show cases of research progress and to discuss the future research directions in these areas.

In the following discussion, we start from the role of simulation in the stability analysis in the power grid. The dynamics of a power grid usually involves alternating currents which are described in nature by sinusoidal signals with a single or multiple frequencies. Using the concept of phasor, which is basically a complex number with a real part and an imaginary part, differential equations of such periodic signals in the steady state may be transferred into algebraic equations in the complex domain. The behavior of the devices in a power grid may be best described in very different time resolutions, typically from microseconds up to seconds or even minutes. Therefore a detailed simulation of such system involves dynamics in multiple time scales. This is known as the curse of stiffness. We will review existing methods to address this unique challenge in such simulation problems in section 2.

A well-known problem in the economic operation of the power grid is the unit-commitment (UC) problem, in which one tries to dispatch the power generation to satisfy the demand from the users with the minimal cost. From a simulation optimization perspective, a unique feature is the presence of system dynamics across multiple spatial resolutions. When the future generation of the renewables and demand from the users are forecast, the UC problems is usually formulated as a mixed integer linear programming (MILP) problem, and solved by Lagrangian relaxations. When many generators are involved, the solution of the LR involves two iterative steps, namely first the optimization giving the multipliers and second the update of the multipliers. This first step may be solved in a decentralized way, each of which addresses a sub-problem. By exploring the similarity among these subproblems, the solution process may be replaced by the approximation given by a neural network, which may be trained and learned from historical data. We will review related work to explore such similarity across multiple spatial resolutions in section 3.

During the evaluation of control policies in autonomous driving, the safety is of crucial importance. However, the safety of a control policy may be affected by random events that occur with very small probabilities. How to effectively evaluate the safety of a control policy by simulation? This is known as the curse of rarity, or the challenge posed by rare events. Typical methods may explore the problem structure to outline a set of representative scenarios and then to test the safety probability in each of these scenarios. We will review related research progress in this field for simulation based safety evaluation of autonomous driving policies in section 4.

The aforementioned stiffness across multiple temporal scales, the dynamics across multiple spatial resolutions, and the curse of rarity are typical challenges that one may face in the simulation of critical infrastructures. We will briefly conclude in section 5.

2 ELECTRIC POWER SYSTEM - STABILITY ANALYSIS

There are dynamics across multiple temporal scales in the electric power grid. To cope with this challenge, both phasor and time domain simulation and analysis have been developed.

2.1 Phasor-domain Simulation

2.1.1 Current Research Status

Dynamic Phasor Method is a new type of system simulation technique, which is an extension of the concept of steady-state phasor. The dynamic phasor $X(t)$ of signal $x(t)$ is defined as (Strunz 2013) $X(t) = \hat{x}(t)\mathrm{e}^{-\mathrm{j}\omega_{\mathrm{s}}t}$, where ω_{s} is a non-negative constant, and $\hat{x}(t)$ is the analytic signal of the signal $x(t)$, satisfying the relationship between the Fourier transforms of the two signals, $x_F(\omega)$ and $\hat{x}_F(\omega)$:

$$\hat{x}_{\mathrm{F}}(\omega) = \begin{cases} 2x_{\mathrm{F}}(\omega) & \omega > 0 \\ 0 & \omega < 0 \end{cases} \tag{1}$$

The property of zeroing the negative frequency in the analytic signal facilitates frequency reduction through frequency shifting, simplifying computation and analysis. When the signal exhibits properties of spectral concentration, numerical computation of the dynamic phasor is more convenient than directly calculating of the original time-domain signal.

Sander (Sanders et al. 1990) proposed an averaging method for analyzing power electronic circuits from the perspective of time-varying Fourier coefficients and applied it to numerical simulation of power electronic circuits. Subsequently, this method was referred to as the dynamic phasor method. Demarcg (DeMarco 1993) defined the dynamic phasor of various orders from the spectrum perspective under certain restrictions on the signal spectrum, and used fundamental frequency the dynamic phasor for numerical simulation of single-machine infinite systems. Venkatasubramanian (Venkatasubramanian 1994) defined the dynamic phasor as the analytic signal of the original signal shifted the synchronous angular frequency on the spectrum when the signal spectrum met the spectral concentration condition.

In AC circuit analysis, the steady-state phasor method is widely employed. The steady-state phasor is a special case of the dynamic phasor. The steady-state phasor method performs calculations in the frequency domain, eliminating the time-varying component $e^{\mathrm{j}\omega_0 t}$ from the time-domain signals, thereby simplifying the equations into time-independent complex algebraic forms, significantly streamlining the computations (Qi 2004). For a single-frequency sinusoidal signal, its instantaneous waveform is a sinusoidal curve, with its envelope waveform being a time-invariant straight line. Consequently, the magnitude of the dynamic phasor represents the envelope of the sinusoidal curve, while the phase of the dynamic phasor corresponds to the phase of the sinusoidal signal. Hence, the dynamic phasor can also be referred to as the complex envelope of the original signal.

For non-sinusoidal periodic excitations in linear time-invariant circuits, the superposition theorem holds, allowing for Fourier series decomposition of the input signal. Each harmonic component is then analyzed separately, and the results are summed to obtain the circuit's full response, the method known as the phasor method. Obviously, a higher number of harmonics leads to more accurate results. Both fundamental and harmonic load flow analyses in power system steady-state analysis employ this approach. However, for aperiodic signals, the waveform of the signal $x(t)$ during the time period $[t-T,t]$ is extended left and right along the time axis of the period T to obtain a periodic signal, and its Fourier expansion is performed on the time window $[t-T,t]$. During expansion, t is a parameter, resulting in coefficients of $e^{jk\omega_0\tau}$ containing the time parameter t. The magnitude and phase of the dynamic phasor for aperiodic signals become functions of time, with the envelope no longer being a horizontal line. As t continuously changes, the dynamic phasor of the original signal varies with time, distinguishing it fundamentally from the steady-state phasor. However, determining the fundamental frequency ω_0 becomes challenging when the aperiodic signal is poorly understood. Furthermore, the lack of a property where later terms are smaller than earlier terms, as observed in Taylor series, makes it difficult to identify which harmonics are the main components of the signal. This makes it difficult to analyze the stage error of the Fourier series, i.e., for certain computational accuracy requirements, it is impossible to determine the dynamic phasor order to be taken. Then the utilization of dynamic phasors is difficult. For power systems, the fundamental components of various electrical quantities are determinate, and there exists a qualitative understanding of the spectral distribution of electrical quantities within the system. Hence, the dynamic phasor method holds an advantage in terms of analytical efficiency.

Compared to time-domain simulation, dynamic phasor calculation allows the use of larger integration step sizes. In contrast to traditional steady-state phasor methods in electromechanical transient simulations, dynamic phasor methods consider a broader range of dynamic phasor orders, thereby enhancing computational accuracy. While increasing the order of the dynamic phasor results in increased computational workload, enlarging the integration step size reduces computational burden. Balancing between these factors can lead to improved computational efficiency.

The Harmonic Balance method (HB) utilizes the concept of the dynamic phasor to solve for the steady-state periodic solutions of a system. A regular periodic solution of an ordinary or differential-algebraic equation system can be represented by a Fourier series, i. e. , a combination of sinusoids. In many cases, a reasonably accurate approximation is already achieved when only a small number of sinusoids is considered (Krack and Gross 2019). In the case of linear differential equations, HB yields a linear algebraic equation system, the solution of which can usually be given as closed-form expression. In the nonlinear case, the algebraic equation system is nonlinear as well, and HB only yields an approximation. However, the essence of HB relies on the Fourier series expansion of nonlinear terms. Therefore, it is constrained by the solution of polynomial-type nonlinear systems (Dai et al. 2024). The harmonic balance method is difficult to apply to complex nonlinear problems that are non-polynomial in nature.

For solving non-polynomial-type nonlinear systems, the HB-Taylor method approximates nonlinear functions with finite-order polynomial expansions using Taylor series (Beléndez et al. 2006). The Alternating FrequencyÍCTime Harmonic Balance method (ATF-HB) approximates the original problem by sampling the temporal values of nonlinear terms and employing discrete Fourier transform (Cochelin and Vergez 2008). HB-recast, proposed by Cochelin et al., is an indirect method that transforms complex nonlinear differential dynamic systems into polynomial-type differential algebraic equations without loss using recasting techniques (Cochelin and Vergez 2008). Wu et al., based on the idea of prediction-correction, improved the Harmonic Balance method by integrating it with the Newton method (Wu et al. 2019).

HB is widely used in solving periodic solutions of nonlinear systems. However, as a semi-analytical and semi-numerical method, the derivation of equations becomes challenging with increasing system degrees of freedom and method orders (Yan et al. 2023). Hall et al. proposed the High-Dimensional Harmonic Balance method (HDHB), which simplifies equation derivation by approximating time-domain calculations of frequency-domain nonlinear terms (Hall et al. 2002). However, the introduction of approximation relationships may lead to non-physical false solutions (Liu et al. 2006; Labryer and Attar 2009). Dai et al. discovered a conditionally equivalent identity between frequency-domain and time-domain nonlinear terms. Based on this, they pioneered the Reconstruction Harmonic Balance method (RHB) to achieve ultra-high-order ($N > 100$) high-precision computations. They also provided an optimal sampling theorem for time-domain collocation calculations, theoretically eliminating non-physical solutions (Dai et al. 2022).

2.1.2 Future Research Directions

In transient simulation calculation of power systems, the Harmonic Balance method can be applied to solve the steady-state solutions of electrical quantities in the power system. HB provides initial steady-state periodic solutions for electromagnetic transient simulations, improving computational efficiency.

For a general device model, its differential-algebraic equation (DAE) system can be expressed as:

$$\begin{cases} \boldsymbol{T}\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{v}) \\ \boldsymbol{i} = \boldsymbol{g}(\boldsymbol{x}, \boldsymbol{v}) \end{cases} \tag{2}$$

where $\boldsymbol{x} \in \mathbb{R}^n$ represents the state variables, $\boldsymbol{v} = [v_a, v_b, v_c]^T \in \mathbb{R}^3$ denotes the terminal voltages of the device, $\boldsymbol{i} = [i_a, i_b, i_c]^T \in \mathbb{R}^3$ is the current injected into the grid by the device, $\boldsymbol{T} \in \mathbb{R}^{n\times n}$ is the coefficient matrix of state variables, $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^n$is the differential equation function of $\boldsymbol{x}$ and $\boldsymbol{v}$, and $\boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^3$is the algebraic equation function computing $\boldsymbol{i}$. We assume that $\boldsymbol{x}(t)$, $\boldsymbol{v}(t)$, and $\boldsymbol{i}(t)$ are all periodic functions with period T. Taking $\boldsymbol{x}(t)$ as an example, it can be expressed using a Fourier series as follows

$$\boldsymbol{x}(t) = \boldsymbol{h}^T(\Omega t)\hat{\boldsymbol{X}} + \boldsymbol{h}^H(\Omega t)\hat{\boldsymbol{X}}^* \tag{3}$$

where

$$\boldsymbol{h}(\Omega t) = \left[1, \mathrm{e}^{\mathrm{i}\Omega t}, \mathrm{e}^{\mathrm{i}2\Omega t}, \cdots, \mathrm{e}^{\mathrm{i}k\Omega t}\right]^T \in \mathbb{C}^{H+1} \tag{4a}$$

$$\hat{\boldsymbol{X}} = [\hat{\boldsymbol{x}}(0), \hat{\boldsymbol{x}}(1), \cdots, \hat{\boldsymbol{x}}(H)]^T \in \mathbb{C}^{(H+1)\times n} \tag{4b}$$

where H represents the maximum harmonic order, $\Omega = \frac{2\pi}{T}$ is the fundamental frequency, $\hat{\boldsymbol{x}}(k)$ denotes the Fourier coefficients, and $\mathrm{e}^{\mathrm{i}k\Omega t}$ represents the Fourier basis function. Taking the derivative of Equation (3), denoted as $\dot{\boldsymbol{X}}(t)$, and substituting Equations (4a) and (4b), we can express it in matrix form as follows:

$$\dot{\boldsymbol{X}}(t) = (\nabla h(\Omega t))^T\hat{\boldsymbol{X}} + (\nabla h(\Omega t))^H\hat{\boldsymbol{X}}^* \tag{5}$$

where $\nabla = \mathrm{diag}(1, \mathrm{i}\Omega, \mathrm{i}2\Omega, \cdots, \mathrm{i}H\Omega)$ represents the diagonal derivative matrix operator. Substituting E-quation (5) into Equation (2), we obtain:

$$\begin{cases} \boldsymbol{T}\left((\nabla h(\Omega t))^T\hat{\boldsymbol{X}} + (\nabla h(\Omega t))^H\hat{\boldsymbol{X}}^*\right) \\ = \boldsymbol{f}\left(\boldsymbol{h}^T(\Omega t)\hat{\boldsymbol{X}} + \boldsymbol{h}^H(\Omega t)\hat{\boldsymbol{X}}^*, \boldsymbol{h}^T(\Omega t)\hat{\boldsymbol{V}} + \boldsymbol{h}^H(\Omega t)\hat{\boldsymbol{X}}^*\right) \\ \boldsymbol{h}^T(\Omega t)\hat{\boldsymbol{I}} + \boldsymbol{h}^H(\Omega t)\hat{\boldsymbol{I}}^* \\ = \boldsymbol{g}\left(\boldsymbol{h}^T(\Omega t)\hat{\boldsymbol{X}} + \boldsymbol{h}^H(\Omega t)\hat{\boldsymbol{X}}^*, \boldsymbol{h}^T(\Omega t)\hat{\boldsymbol{V}} + \boldsymbol{h}^H(\Omega t)\hat{\boldsymbol{X}}^*\right) \end{cases} \tag{6}$$

In the Harmonic Balance method, Equation (6) is typically solved by equating the Fourier series in each term. However, in practical engineering applications, models of devices often involve nonlinear functions, making it difficult to obtain Fourier series expressions that decouple each harmonic. In such cases, ATF-HB can be adopted, where discrete Fourier transform are used to approximate the Fourier coefficients.

2.2 Time-domain Simulation

The main goal of a time domain simulation is to determine if there is a bounded trajectory of the system toward an equilibrium point following a disturbance (Ma and Zhang 2023). Determining the level of modeling detail required to capture the particular phenomena of interest accurately is key when developing a power systems simulation model. Electromagnetic transient (EMT) simulation is a vital tool for studying complex transient behavior. It spans the timescale from microseconds to milliseconds, over which the dynamics of wave propagation, switching surges, inverted-based controls, stator transients and sub-synchronous resonance interact with both electromechanical and electromagnetic phenomena (Lara et al. 2024). The objective of this section is to provide an overview of modelling techniques and computation methods implemented in industry applications as well as academic research.

2.2.1 Network and Device Modelling

The device and network modelsąŕ level of detail determines the requirements placed on time-domain simulation solution methods. For EMT specifically, both network and device dynamics should be considered.

The network circuit dynamics in the EMT simulation is distinct from those in electromechanical phenomena. The detailed dynamic model of a transmission line is Telegrapher's equations using Partial Differential Equations (PDEs) for the voltage and current across the line length with distributed parameters. However, it is difficult to include this level of detail in time-domain simulation tools, and experience shows that the impacts of using simplified models are not significant for most applications. The common simplification is the lossless line assumption, i.e. the resistance and conductance per unit length are zero, which results in a simplified two-port model interfaced via a current source with constant time delay. The Dommel line model (Dommel 1969) extends the delayed current-source model approximating the series resistance losses by adding lumped resistances at both ends and middle of the two-port system.

A typical application in device level EMT simulation is synchronous generators. The foundation for modeling synchronous generators can be traced back to the early years of the 20th century, as highlighted in references (Park 1929; Park 1933). Two prominent approaches, namely the two-reaction theory and the Park transformation, have played pivotal roles in this historical development. To a large extent, contemporary practices in generator modeling have evolved from the seminal works of Blondel and Park. The resulting machine model is described sets of nonlinear ordinary differential equations (ODEs), composed of stator and rotor voltage equations, rotor flux linkage equations, and the rotor swing dynamics. One common simplification is to set the derivative of stator magnetic flux ψ to zero. The simplification implies that the terms ψ decay very rapidly after a perturbation, as observed in practice (Anderson and Fouad 2003). This simplification also removes high frequency transients and fundamental frequency components in the d-axis and q-axis stator currents, which in turn also allows larger time steps in the simulation execution.

Another class of devices that completely differs in their energy conversion mechanism from synchronous generators is Inverter Based Resources (IBR). Instead of using a rotational magnetic field, IBRs synthesizes voltages through high frequency switching, introducing high-frequency dynamics into the synthesized voltages and realized currents. Despite the high-frequency behavior, IBRs include output filters and controllers with low-pass filters tuned to regulate average values (Yazdani and Iravani 2010). These aspects readily provide the rationale to disregard switching-level dynamics from IBR models intended for system-level studies (Martinez-Velasco 2015). From the perspective of EMT modeling objectives, the main challenge arises from the network topology and conductivity matrix changes caused by the numerous switching actions. The currently mainstream modeling approaches are mainly classified into two classes: topology modeling method and external characteristics based modeling method. The former is subdivided into ON/OFF model, R_{ON}/R_{OFF} model (Woodford et al. 2015), Transmission line model (TLM) and L/C model (Sudha et al. 1993), according to the internal topology structure of power electronic switches dynamics. The latter integrates the power electronic device and equivalently represents it as a multi-port network. The performance of switch models needs to be verified against equipment behavior before integration into existing software tools.

2.2.2 Computation Methods

The EMT simulation represents the full wave throughout the entire process, which results in a time-variant model. As a result, these models require special consideration when choosing integration techniques. The most developed software solutions for EMT simulations employ the numerical integration substitution technique with a trapezoidal rule for integration as originally developed by Dommel (Dommel and Sato 1972) to simulate circuit behavior. Examples of software environments are PSCAD, EMTP, DIgSILENT PowerFactory, among others. The ultimate objectives are set to maximize computational speed and modeling precision (Mahseredjian et al. 2009). To achieve trade-off between them, several factors are typically considered when constructing numerical integration.

Firstly, the approximation accuracy and computational cost of a numerical integration method depend on the step size h and the integration method order $\mathscr{O}(h^n),\ n > 1$. Reducing h can improve accuracy by reducing the relative importance of high-order terms, but it comes at the expense of more algorithm iterations. According to Corless and Fillion (2013), if the largest error tolerated within a single iteration is 10^{-n}, it is best to choose at least a nth order algorithm.

Secondly, the stiffness of models. Although there is no widely accepted definition of model stiffness, a classical measure is the stiffness ratio s, defined as (Eshkabilov 2020) $s = \frac{\max_{\forall i} |\sigma_i|}{\min_{\forall i} |\sigma_i|}$, where σ_i is the real part of the ith eigenvalues. When $s > 10$, the equation can be considered stiff. The challenges of simulating systems with IBRs stem from interactions across time scales, and the requirements to include fast electromagnetic dynamics increases model stiffness further. Therefore, it becomes imperative for the chosen numerical integrator to navigate through stiff regions. Explicit integration methods, like Runge-Kutta, have difficulty coping with highly stiff simulation models that result from the simultaneous modeling of electromechanical and electromagnetic phenomena. While implicit numerical integration methods can overcome explicit methodsą́ challenges with stiff systems, like trapezoidal method mentioned earlier.

In addition to conventional numerical integration methods based on Taylor approximation, recent developments in the field of power system EMT simulation have introduced method known as *geometric numerical integration*. Generally, the conventional integration methods do not exploit the underlying structure of the system, and consequently some physical properties may be distorted or even lost, adversely affecting the dynamic behaviour of the system during the numerical integration process. The most notable phenomenon is the spurious energy introduced during the time discretization and numerical integration process (Hairer et al. 2006), which degrades the numerical stability and solution accuracy. To solve this problem, numerical integrators for preserving the underlying physical invariant have emerged. If certain energy function is preserved along the discretized trajectories, the numerical integration methods are called geometric numerical integrators with exact energy conservation. In general, there have been three classes of geometric numerical methods developed so far that can achieve exact energy conservation, namely the collocation method (Kotyczka and Lefĺĺvre 2019), the splitting method (McLachlan et al. 2002), and the discrete gradient method (Schulze 2023). The first two methods are restricted to linear Hamiltonian systems, which are obviously not applicable to the nonlinear synchronous generator models. The discrete gradient method, though initially limited to linear Hamiltonian systems in astrophysics (Dahlby et al. 2011) and classical mechanics (Liu et al. 2013) to preserve multiple invariants, is recently applied to nonlinear systems (Budd et al. 1999) and shows excellent exact energy conservation performance. The extension and application of the geometric numerical integration to nonlinear power system EMT simulation is very limited. A major reason is the difficulty to reconstruct power system component models into canonical *port-Hamiltonian form*, i.e. a type of special representation that follows the original geometric structure .

3 SMART GRID - SUPPLY DEMAND MATCHING

From simulation optimization perspective, a unique feature of supply demand matching in smart grid is the presence of multiple agents, and the system dynamics across multiple spatial scales. And lots of problems in the power system could be formulated as Markov decision process (MDP) problems. We use reinforcement learning (RL) to address the MDP problems and take the unique feature of supply demand matching requirements into account to develop as series of efficient algorithms. For the large-scale centralized problems, we use Lagrangian relaxation to handle the supply demand matching requirements.

For the distributed microgrid problems, we use distributed multi-agent RL to address matching requirements and constraints across multiple spatial scales.

3.1 Large-scale Unit Commitment Problems

With the extensive integration of renewable energy, power systems increasingly need to manage variability, which requires enhanced real-time capabilities in system planning. Effectively solving unit commitment (UC) problems are essential for power system operators. The UC problems are commonly formulated as mixed integer programming (MIP) problems and the industrial-scale UC problems are typically solved using commercial solvers such as CPLEX or GUROBI which uses advanced Branch-and-Cut or Branch-and-Bound algorithms (Ostrowski et al. 2011). However, the performance of these solvers is far from satisfying in large-scale UC problems. Surrogate Lagrangian relaxation (SLR) methods (Bragin et al. 2015) have been used for large-scale UC problems (Sun et al. 2018; Wu et al. 2021). SLR divides the UC problem into independent sub-problems for each unit that can be solved more rapidly by Lagrangian relaxation and SLR updates the Lagrangian multipliers iteratively using their surrogate sub-gradients that are obtained by solving some sub-problems. SLR can obtain a good enough solution of the large-scale UC problem than commercial solvers, but it still faces challenges that it requires repetitive solving of similar sub-problems iterations which reduces overall efficiency.

We proposed a reinforcement learning embedded surrogate Lagrangian relaxation (RL+SLR) method for fast solving UC problems (Zhu et al. 2024). RL+SLR can swiftly solve the sub-problems for one unit under varying Lagrangian multipliers because it formulate the sub-problems associated with each unit as an MDP problem and apply RL to learn the optimal policy which can provide a near-optimal unit state sequence under various Lagrangian multipliers. In the MDP of unit i at time t, the state $s_{i,t}$ consists of the unit on or off state, unit output power, open or close hold time and "penalty price" sequence $W_{i,t}$. $W_{i,t}$ consists of ąřpenalty pricesąś $w_{i,t}$ from the current time t to T, with zeros appended at the end to maintain constant dimensionality. The variable $w_{i,t}$ is obtained through a weighted sum of Lagrangian multipliers, which represents the incremental cost of the power output of the unit in the Lagrangian relaxation problem under the current values of the multipliers. The formal definition is as follows

$$w_{i,t} = (\mu_t + \sum_{l \in N_L} (\lambda_{l,t} - \kappa_{l,t}) \Gamma^G_{l,i}), W_{i,t} = (w_{i,t}, w_{i,t+1}, \cdots, w_{i,T}, \overbrace{0, \cdots, 0}^{t-1})^T, \tag{7}$$

where μ_t is the Lagrangian multiplier of the supply demand matching constraints, and $\lambda_{l,t}, \kappa_{l,t}$ are the Lagrangian multipliers of the upper and lower transmission capacity constraints for line l at time t. In the MDP, the action for unit i involves changes in the on or off status and power output. We utilize a deep Q networt to train agents for each unit offline, which is then used online to solve each sub-problem.

After training the Q-function for each unit, the UC problem can be solved by RL+SLR, which uses SLR as the framework and uses RL to solve the sub-problems in the iteration of SLR. The traditional SLR method uses the commercial solver to solve sub-problems. In RL+SLR, we can obtain near-optimal solutions of the sub-problems of unit i under various Lagrangian multipliers by doing only T forward propagation computations in the well-trained Q-function. The time complexity for solving a sub-problem is $\mathscr{O}(T)$ and it is not affected by the form of the function of fuel cost.

Table 1 shows the results of the three large-scale sub-hourly UC problems for the 10K-bus system (Birchfield et al. 2017). RL+SLR can obtain a feasible near-optimal solution with no more than 3% performance degradation, but $25 \sim 110$ times faster than Gurobi, and also $3 \sim 4$ times faster than SLR.

3.2 Microgrids Problems

In this section, the Microgrids (MG) are considered to cooperatively minimize the total electricity cost while maintaining voltage safety. The overall structure of the multi-MG system is shown in Figure 1. The

Table 1: 10k-bus system T=96 (adapted from Zhu et al. (2024)).

Problem	Units	Method	Object ($)	t_{iter} (s)	t_{CPU} (s)	Gap
P1	1136	Gurobi[a]	37865029	–	13607	–
		Gurobi[b]	28618236	–	14712	–
		SLR	28783083	1095	1398	0.58%
		RL+SLR	29441396	132	543	2.88%
P2	1086	Gurobi[a]	26706896	–	9084	–
		Gurobi[b]	26680023	–	23775	–
		SLR	26833562	1149	1330	0.57%
		RL+SLR	27362916	134	289	2.56%
P3	1044	Gurobi[a]	32953504	–	17889	–
		Gurobi[b]	25640281	–	41178	–
		SLR	25809754	1187	1564	0.66%
		RL+SLR	26235824	126	374	2.32%

[a] The first feasible solution found by Gurobi.
[b] A good feasible solution found by Gurobi.

MGs are connected to the distribution network and the power flow is bi-directional. The distribution also exchanges power with the high voltage grid. Each MG owns power loads and distributed energy resources. The MGs cooperatively minimize the total electricity cost of the entire distribution system. Meanwhile, the MGs need to ensure the safety of the power grid, which is to limit the nodal voltage within the safe range. There are some on-line algorithms such as the on-line alternating direction method of multipliers (ADMM) are applied to dispatch the MGs in real time (Ma et al. 2016). However, these algorithms usually depend on the simplified mathematical models, like linear power flow equations, and only make one-step iteration for speed improvement. And these methods are model-based that require the MGs and the operator to have an accurate closed-form model of the distribution network and the electrical devices, which might be hard to obtain due to privacy concerns and information scarcity.

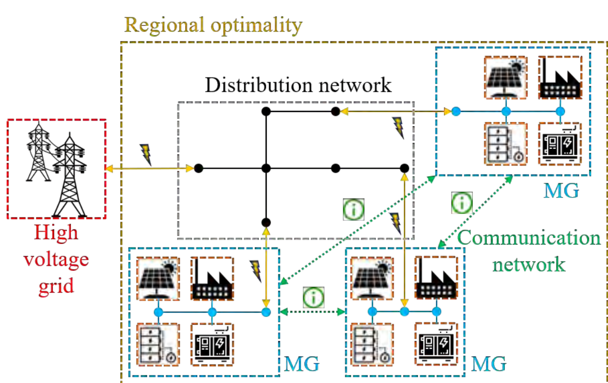

Figure 1: The framework of the multi-MG system (adapted from Cui et al. (2024b)).

Because the economic dispatch problem belongs to the tertiary control in the power system (Chen et al. 2020). The low-frequent violation of the voltage constraint could be tolerated in practice, which would be handled by the secondary control system (Fan et al. 2021; Xu et al. 2021). Thus, we relax the voltage constraint as a chance constraint (Chen et al. 2022) and the energy management problem of the multi-MG system as a constrained multi-agent Markov decision process (CMAMDP). And we propose a distributed

RL algorithm with a convergence guarantee to solve the general CMAMDP, which could preserve private information about local costs. To improve the performance and further preserve the privacy of local states and actions, we develop the feature extraction module based on deep neural networks which will encrypt the local state-action pairs, and we incorporate this module into the algorithm (Cui et al. 2024b).

We do the numerical experiments on the two distribution networks with 4 and 8 MGs. The experimental results demonstrate that our algorithm outperforms the existing methods including the interior point method and on-line ADMM in regulating the frequency of voltage violations. This regulation is at the expense of 1-2% higher economic cost in the experiments. Compared against the RL algorithm with fixed penalizing term, our algorithm is adaptive to various preset limits. And our algorithm could preserve the local privacy of each MG, and thus is more applicable in the real system.

3.3 Microgrids Real-time Pricing

In this section, we consider coordinate the MGs in the distribution network by setting prices as incentive signals. Because of the high uncertainty of loads and renewable resources, it is necessary for the distribution system operator (DSO) to adopt real-time prices. MGs will make the generation plans by the reference price sequences set by DSO. The pricing task is generally modeled as a bi-level optimization problem (Alam et al. 2018). At the upper level, the DSO decides the reference price sequence. At the lower level, the MG makes its generation plan for the received reference prices. This bi-level optimization problem could be transformed into a mixed-integer linear programming (MILP) problem using the KarushÍCKuhnÍCTucker (KKT) conditions and solved by commercial solvers (Toutounchi et al. 2019). However, due to privacy concerns in practice, the MGs may not provide adequate information for the DSO to build a closed-form model, which causes challenges to the implementation of the conventional model-based methods.

We transform the above problem into a MDP and solve it by the model-free RL that optimizes the DSO pricing policy by learning from experience (Cui et al. 2024a). In this way, DSO could optimize the pricing policy when the response behavior of the MGs is unknown. However, the action dimension of the MDP problem is to high. For example, if the price sequences for 4 MGs are generated for the next 24 hours divided into 5 minutes, the cardinality of the action space would be 1152, which caused the agent hard to reach an optimized policy. To address this problem, we propose to incorporate a reference policy into the regular RL algorithm. The reference policy we set could be generated easily when the prediction for the real-time prices of the high voltage network is obtained and it could assist the agent to generate a reasonable policy at the beginning of training.

We do the numerical experiments on the 4 and 8 MGs in the IEEE 33-node distribution network. We also consider two situations that these problems are transformed into MILP and mixed-integer quadratic programming (MIQP) by KKT conditions. The results are demonstrated in TABLE 2 and 3. “Baseline” is using Gurobi to solved the MILP or MIQP problems, which knows the complete information. Our algorithm performs almost as well as the model-based method and is more practical by privacy preservation for the MGs. And the results show that our algorithm is also effective when the MGs consider quadratic cost functions and (dis)charging loss.

Table 2: Comparison of cost (U.S. $/5 minutes) of the DSO with the problem transformed as MILP.

MG number	Initial policy	Reference policy	Our algorithm	Baseline
4	400.06	352.18	323.32	317.13
8	404.04	286.57	240.35	228.14

Table 3: Comparison of cost (U.S. $/5 minutes) of the DSO with the problem transformed as MIQP.

MG number	Initial policy	Reference policy	Our algorithm	Baseline
4	409.67	373.45	346.38	338.71
8	315.57	284.59	255.82	245.26

4 AUTONOMOUS DRIVING - EFFICIENT SIMULATION AND ANALYSIS

Curse of Rarity (Liu and Feng 2022) has been a significant long-standing problem for the simulation of autonomous vehicles (AVs). Safety-critical events occur infrequently within high-dimensional variable spaces, and the majority of existing data offers minimal insight into these rare occurrences. Meanwhile, as the safety performance of AV improves, such situations become even scarcer, intensifying the Curse of Rarity issue. The rarity creates distinguished challenges for accurately and efficiently simulating AVs and analyzing their safety performance. For instance, it can bring severe data imbalance in safety-critical perception tasks of AVs, hinder precise behavior modeling for both AVs and background vehicles(BVs) in safety-critical situations, lead to severe policy gradient estimation variance for learning decision-making models, and result in dramatic variance for AV testing. Consequently, addressing the safety-critical components in these aspects of AVs, particularly in AV testing, is challenging. At present, there are primarily two methods for AV testing, including scenario-based approaches and environment-based approaches.

4.1 Scenario-based Simulation

Scenario-based approaches aim to test AVs in specially crafted scenarios that emphasize safety-critical situations. How to design and generate such scenarios, however, remains an open question, and many approaches have been developed, including combination-based scenario generation, worst-case scenario generation, adaptive scenario generation, and likely-failure scenario generation. The combination-based scenario generation approach (Zhou and del Re 2017) introduces permutation and combination logic, which fundamentally decomposes scenarios into several basic scenario units and constructs complex scenarios by permuting and combining these basic units. The worst-case scenario generation approach (Jung et al. 2007) is to generate the most challenging scenarios for AVs. For instance, Ma et al. utilize game theory methods to optimize the interference factors in scenarios, generating scenarios most likely to cause rollover or hard braking of AVs (Ma 1998; Ma and Peng 1999). The adaptive scenario generation approach calibrates the AV surrogate model gradually through dynamic testing to explore and determine the model's effectiveness boundaries, generating representative scenarios. For example, Mullins et al. utilize an adaptive testing scenario search algorithm to gradually discover the model's effectiveness boundaries and provide corresponding test scenarios to measure its safety performance (Mullins et al. 2018). The likely-failure scenario generation approach aims to discover the most likely scenario that causes failure to determine the AV's failure boundary. Koren et al. (Koren et al. 2018) apply this method to test the safety of AVs passing through pedestrian crossings, discovering scenarios with a high probability of resulting in collisions.

However, scenario-based approaches face two limitations. Firstly, most existing scenario-based testing methods are only suitable for short scenario segments (typically around 10 seconds), involving a limited number of dynamic objects (e.g., one or two background road users). These scenarios are typically characterized by simple, low-dimensional decision variables. For example, OąŕKelly et al. attempted to extend the scenario-based approach to more complex, high-dimensional scenarios involving five background vehicle (BVs) (O'Kelly et al. 2018). However, an AV operating in an urban area over an extended period could interact with hundreds of other vehicles and road users, performing a variety of maneuvers such as car-following, lane changing, and merging, and navigating diverse road types such as roundabouts and intersections. Current scenario-based methods struggle to handle such complexity. While these short segments are valuable for gauging basic driving skills, they can not adequately assess AV's overall safety performance efficiently (Shladover and Nowakowski 2019).

Secondly, scenario-based approaches typically test AVs on a case-by-case basis, which limits their effectiveness. In contrast, continuous testing of AVs can automatically generate and combine various scenario segments, efficiently uncovering potentially unknown unsafe scenarios. For instance, an AV that performs well in two separate scenario segments might fail when these segments are combined during continuous testing. This failure can occur because, in isolated tests, the AV is optimized to handle specific, controlled conditions. However, when scenarios are combined, the context shifts, rendering previously effective strategies inadequate or inappropriate. The AV must then adapt its strategies to this broader, more complex context. Additionally, it is important to note that most autonomous vehicles (AVs) exhibit non-Markovian behavior in their perception, decision-making, and sometimes control modules. This means that historical data can influence their performance in ongoing tests. Such dependencies can lead to accumulated errors within the AV's systems, which might worsen existing challenges and further complicate performance in continuous testing environments. As pointed out in ISO 21448, unknown unsafe scenarios should be proven to reach a sufficiently low level and comply with quantitative targets for AV validation. Therefore, subjecting AVs to continuous testing in spatially and temporally complex driving environments is essential for comprehensive AV validation, a task beyond the scope of current scenario-based methods.

4.2 Environment-based Simulation

The first prevailing approach to environment-based testing involves driving AVs in naturalistic driving environments (NDE), observing their performance, and making statistical comparisons to human driver performance (Kalra and Paddock 2016). These statistical comparisons, essential for determining the readiness of AVs for widespread deployment (Webb et al. 2020; Shladover and Nowakowski 2019), often quantify safety performance using metrics such as crash rates for various types and severities of crashes per mile driven. These metrics are commonly employed to assess the safety performance of human drivers (Kalra and Paddock 2016). To evaluate the safety performance of AVs, most simulation methods test high-fidelity AV models in life-like simulations of NDE, such as Microsoftąŕs Air-Sim (Shah et al. 2018), Google/Waymoąŕs Car-Craft (Madrigal 2017), Baiduąŕs AADS (Li et al. 2019), etc., where different techniques could be utilized resulting in NDE models with different fidelity. However, these methods are based on historical data replay or using highly simplified physics models and manually designed rules for simulation, which differ significantly from real-world driving environments. Yan et al. further expanded to more complex and highly interactive urban roundabout environments, learning NDE models that statistically match real human driving behaviors (Yan et al. 2023). The main limitation of the NDE-based testing methods lies in the difficulty of learning modeling from real data, resulting in low accuracy and poor interactivity of the obtained NDE models, i.e. the probability distributions are not accurate enough, and there is a lack of interaction between different traffic participants. Therefore, the accuracy of testing results based on this NDE model is affected. Meanwhile, due to the rarity of safety-critical events in NDE, hundreds of millions of miles and sometimes hundreds of billions of miles would be required to demonstrate the safety performance of AVs at the level of human-driven vehicles (Kalra and Paddock 2016; Wachenfeld and Winner 2016), which is intolerably inefficient.

The second environment-based testing approach is based on accelerated environments, which can greatly alleviate the problem of low testing efficiency in the first approach. It increases the sampling probability of safety-critical scenarios to reduce the number of tests while maintaining the unbiasedness of the test results. Zhao et al. introduced importance sampling into autonomous driving testing, utilizing variance reduction techniques on top of Monte-Carlo sampling to increase the occurrence probability of extreme scenarios while ensuring unbiased estimation of sample parameters (Zhao et al. 2016). Since parameterized distributions struggle to accurately fit high-dimensional parameter spaces with spatio-temporal correlations, Zhang et al. introduced normalized flow into the importance sampling method to target the joint distribution of spatio-temporal parameters (Zhang et al. 2022). Feng et al. constructed an accelerated environment for autonomous vehicles based on importance sampling and NDE models, identifying critical background vehicles and changing their action probability distributions to execute highly challenging driving strategies, thereby accelerating the occurrence of safety events (Feng et al. 2021). However, due to the Curse of Rarity problem, safety event information is extremely sparse, making it difficult to design effective challenging driving strategies. Feng et al. further proposed a dense deep reinforcement learning algorithm to identify and remove non-safety-critical data and densify key information for neural networks to learn challenging driving strategies, thereby constructing effective accelerated environments (Feng et al. 2023). The limitation of accelerated environment-based testing methods is the inadequate equivalence of test results with real-world performance. Due to the necessity of accurate real-world probability distributions for effective importance sampling, inaccuracies in NDE models hinder the precision of importance sampling results. As a consequence, accurately reflecting the safety performance of the tested AV becomes challenging (Riedmaier et al. 2020).

4.3 Challenges for Simulation of Autonomous Vehicles

Several challenges must be addressed to fully leverage the environment-based simulation.
Challenge #1: Simulating Normal Driving Behaviors in Realistic and Efficient Ways. Human drivers exhibit a wide range of behaviors influenced by personal traits, mood, experience, and cultural norms. Driving also involves complex interactions among multiple drivers. It is challenging yet important to develop models to capture such subtleties, and in a computationally scalable and efficient way.
Challenge #2: Simulating Rare Driving Behaviors in Safety-Critical Situations. Human drivers exhibit an average accident rate of approximately 1.9×10^{-6} per mile. Safety incident data are therefore scarce in nature. It is challenging yet crucial to generate safety-critical situations.
Challenge #3: Beyond Agent Behavior simulations. Mainstream agent simulations primarily emphasize modeling agent behavior, typically considering environmental factors with short time durations. To create more realistic testing environments for spatio-temporal continuous simulations, it's essential to model the environment dynamics over long time horizon and incorporate BV's more complex interactions with them.
Challenge #4: Enhancing AV Safety Performance with Efficient Feedback Loop. The curse of rarity problem leads to data imbalance, which significantly increases the training difficulty in deep learning models. As AVs achieve better safety performance, the safety-critical events occur even less frequently. It remains open how to model the unknown corner cases that might be missed in simulation but occur during road test.

5 CONCLUSION

In this work we review the state of art in simulation and AI in two critical infrastructure in modern societies, namely the power grid and autonomous driving. Beyond the common requirement on the efficiency of the simulation and the performance of the optimization, each of these systems demonstrate specific challenges and research opportunities for simulation and AI. The stability analysis of power systems involves dynamics in both the phasor and the time domain. The supply demand matching in power grid involves multiple spatial and temporal resolution as well as multiple agents. The efficient evaluation of control policies in autonomous driving needs to address rare events. We wish this work may shed light on the synergy between simulation and AI in critical infrastructures in the near future.

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