Harnessing AI for Energy Transitions

Role of Big Data, Large Language Models, and Agentic Intelligence

Ashkan Safari[1,2], **Afshin Rahimi**[1]

[1] Mechanical, Automotive & Materials Engineering, University of Windsor, Windsor, ON, Canada ({safari8, arahimi}@uwindsor.ca)

[2] Faculty of Electrical and Computer Engineering, University of Tabriz, Tabriz, Iran (ashkansafari@ieee.org)

ORCIDs: {AS:0000-0002-1780-7615, AR: 0000-0002-5737-1385}

Abstract

Climate change is causing unprecedented global warming, rising sea levels, and extreme weather events that threaten ecosystems and human societies worldwide. To combat this and mitigate its impacts, the world is striving for an energy transition towards 100% renewable energy systems and net-zero communities. For this transition, several challenges, such as infrastructure requirements or costs, exist. One of the solutions to cover these challenges is to make the most of digital technologies, especially Artificial Intelligence (AI). AI-driven technologies can improve the design and operation of renewable farms, streamline energy storage solutions, and enable smarter urban planning to lower carbon footprints. Additionally, AI can analyze large amounts of data to identify sustainable practices and support decisions, driving faster progress toward net-zero emissions. However, the more the data increases and becomes larger big data, these classical AI models face challenges in their analytics, especially in real-time operations. To this end, the importance of big data in power systems, and the more advanced AI strategies, known as Large Language Models (LLMs) and agentic AI, are taken into consideration. For both LLMs and agentic AI strategies, one case study is analyzed for each, with several recent literature and recent developments. Then, the challenges and future research directions are presented, supported by the complementary descriptions of these technologies with the United Nations Sustainable Development Goals (UN-SDGs). Harnessing AI's potential in the energy transition through optimized renewables, intelligent grids, and sustainable data centers (to process these AI strategies) can be considerably beneficial for a resilient, net-zero future.

Introduction

The global energy transition, driven by the urgent imperative to mitigate climate change, is affecting the world's energy sector through innovative solutions addressing technical, economic, and social challenges of decarbonization (Li et al., 2025). As rising global temperatures and extreme weather events highlight the consequences of greenhouse gas emissions, nations are accelerating the shift from fossil fuels to fully Renewable Energy Sources (RES) and a net-zero community. Following this urgency, several organizations provided sustainability goals to achieve a net-zero community. One of these organizations is the United Nations (UN), which presented the Sustainable Development Goals (SDG) (Fund, 2015). The other important regulatory agreement is the Paris Agreement. The Paris Agreement, adopted in 2015 under the UN Framework Convention on Climate Change (UNFCCC), is a landmark global treaty aimed at combating climate change by limiting global warming to well below 2°C, ideally 1.5°C, above pre-industrial levels (Bodansky, 2016; Mudhee et al., 2025). Although the RES have proved that they accelerate the transition process to a fully net-zero community, several challenges remain, including the electrification infrastructure and the associated costs (Heuberger & Mac Dowell, 2018; Al-Shetwi et al., 2024; Heptonstall & Gross, 2021). In order to provide solutions for those challenges, Artificial Intelligence (AI) is the strategy that is being focused on (Salman et al., 2024). The reason for this is AI's potential. AI can optimize renewable energy production by predicting weather patterns for solar and wind, improving grid efficiency, and managing energy storage to balance supply and demand (Sankarananth et al., 2023). Additionally, it enhances energy efficiency in industries, buildings, and transportation through predictive maintenance and smart systems (Farzaneh et al., 2021). Moreover, AI accelerates research into new materials for batteries and carbon capture technologies (Priya et al., 2023). By processing vast datasets and enabling real-time decision-making, AI helps reduce costs, lower emissions, and scale clean energy solutions, making it a cornerstone for achieving global climate goals efficiently and effectively (Ukoba et al., 2024). Following this potential, AI in the renewable energy market is considerably increasing, as shown in Fig. 1.

The global AI in renewable energy market is projected to reach approximately USD 78.2 billion by 2034, up from USD 8 billion in 2024, with a Compound Annual Growth Rate (CAGR) of 25.60% from 2025 to 2034. In 2024, the Asia-Pacific region is anticipated to dominate the market, holding over 35% of the market share and generating $2.8 billion in revenue (Market.us, 2025). As mentioned, one of the important applications of AI is in the materials for batteries and carbon capture technologies. Accordingly, Fig. 2 shows the Sankey diagram of the critical minerals in clean energy transitions, which is gathered from (IEA, n.d.).

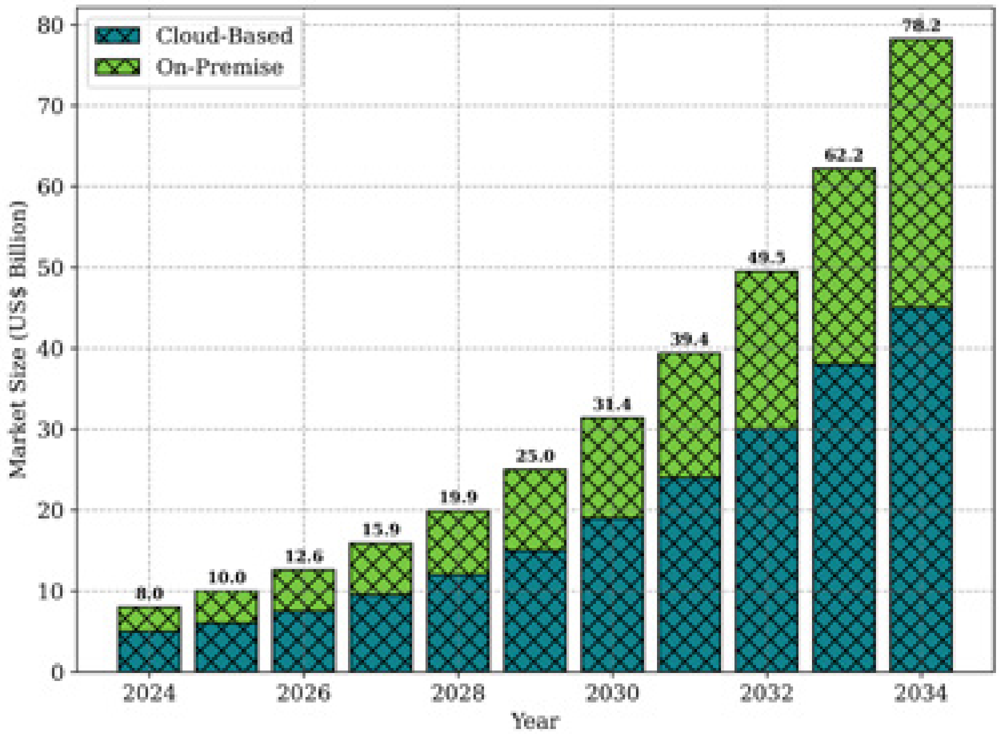

Figure 1: Artificial intelligence in the renewable energy market statistics, based on the data from (Source: Market.us, 2025).

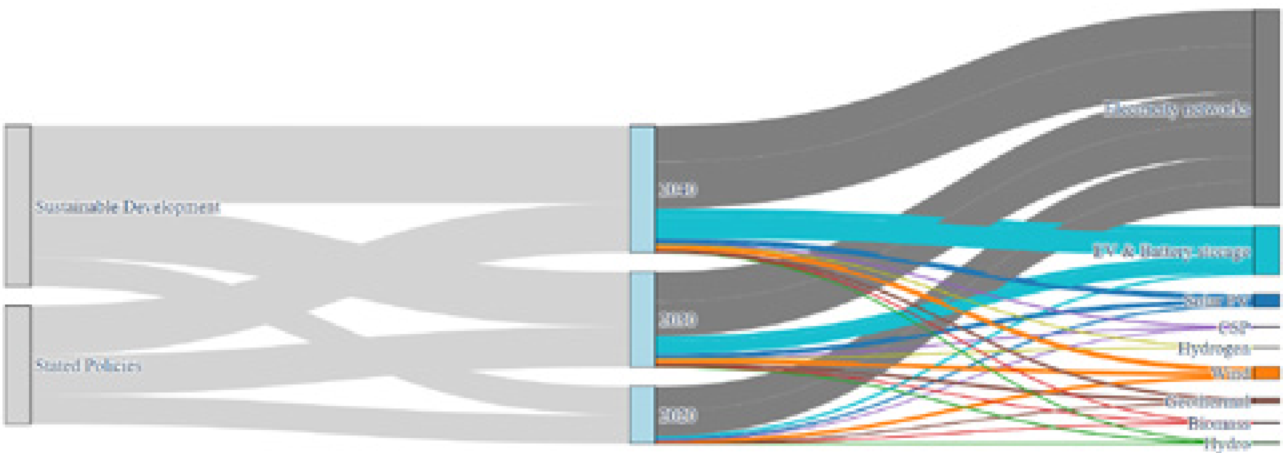

Figure 2: Sankey diagram of critical minerals in different energy technologies, considering sustainable development and policies, based on the data from Source (IEA, n.d.). A Sankey diagram is a flow diagram that visualizes the magnitude of flows between nodes, with arrow widths proportional to the flow quantity.

As reported in (IEA, n.d., IEA, 2021), the types of mineral resources required differ depending on the technology. Lithium, nickel, cobalt, manganese, and graphite are essential for battery performance, durability, and energy density. Rare earth elements are critical for permanent magnets used in wind turbines and Electric Vehicle (EV) motors. Electricity grids rely heavily on copper and aluminium, with copper being a key component in all electricity-related technologies. The transition to a clean energy system is expected to increase the demand for these minerals, positioning the energy sector as a major player in mineral markets. As clean energy transitions accelerate, clean energy technologies are now the fastest-growing source of demand. In a scenario aligned with the Paris Agreement goals, the share of total demand for these minerals is projected to rise sharply over the next two decades: over 40% for copper and rare earth elements, 60-70% for nickel and cobalt, and nearly 90% for lithium. EVs and battery storage have surpassed consumer electronics as the largest consumers of lithium and are expected to overtake stainless steel as the primary end user of nickel by 2040 (IEA, n.d., IEA, 2021). The world is on pace to double the demand for minerals used in clean energy technologies by 2040, according to the IEA's Stated Policies Scenario (STEPS). This surge is driven by the rapid expansion of clean energy systems, with technologies of EVs, battery storage, and renewable energy infrastructure requiring substantial amounts of minerals such as lithium, nickel, cobalt, copper, and rare earth elements. Consequently, AI applications in those economies, environments, and energy, such as Deep Learning (DL), and Machine Learning (ML) strategies, find importance, as reviewed in (Sarwar et al., 2024).

To this end, in this article, we have emphasized the role of harnessing AI in energy transition by presenting the importance, applications, and use cases of big data, Large Language Models (LLMs), and agentic AI in power systems. Firstly, the big data and its different usage strategies in power systems are presented in Section 2. Then, LLMs are described and one of their case studies in power systems, and several literatures in that field (Section 3). As the LLMs and their insights are presented, Section 4 describes the agentic AI concept, a case study, and the relevant literature. Next, the challenges, associated future works, and the alignment with UN SDGs are given in Section 5. Finally, the conclusion is drawn in Section 6.

Big data in power systems

The power sector generates vast amounts of data from sources, such as smart meters (Wen et al., 2018, Alemazkoor et al., 2022), sensors (Rani et al., 2017, Marinakis et al., 2020) on grid infrastructure (Munshi & Yasser, 2017), renewable energy systems (Mostafa et al., 2022, Ejiyi et al., 2025), and consumer devices (Al-Ali et al., 2018, Hu & Vasilakos, 2016), characterized by high volume, velocity, and variety (which are the three Vs of big data). This data is important for real-time monitoring and predictive maintenance, allowing utilities to detect equipment failures before they occur, thus reducing outages and maintenance costs. Big data analytics also facilitates the integration of renewable energy sources, such as solar and wind, by analyzing weather patterns and consumption trends to balance supply and demand, optimizing grid stability (Safari et al., 2024). Furthermore, it supports demand-side management through insights from consumer usage patterns, enabling dynamic pricing and energy-saving recommendations. By extracting information from complex datasets, big data empowers power systems to meet growing energy demands, reduce carbon footprints, and transition toward a more sustainable and intelligent energy ecosystem. Following this importance, big data can be used in different aspects of power systems. These aspects are presented in Fig. 3 (Guo et al., 2018).

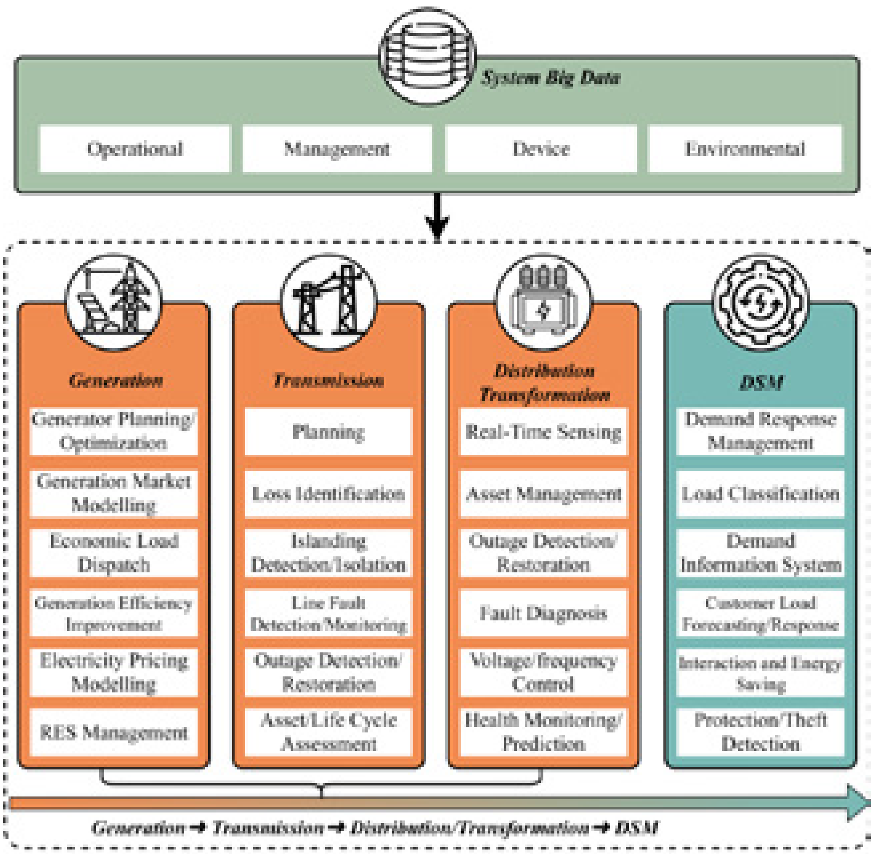

Figure 3: Big data application in power systems different sections: From Generation to Demand Side Management (DSM) (Source: Guo et al., 2018)

Based on (Guo et al., 2018), power system big data is categorized into four dimensions: operational, management, device, and environmental. In power generation, big data can be used for optimizing resources and achieving cost efficiency. It supports applications such as generator planning and optimization, market modeling, and economic load dispatch, helping utilities balance supply and demand effectively. Additionally, big data-based analytics can improve generation efficiency, electricity pricing models, and RES management. In the transmission sector, big data enhances both planning and real-time operations. It enables applications such as loss identification, islanding detection and isolation, and line fault detection and monitoring, ensuring stable power transmission over long distances. Additionally, big data supports outage detection and restoration, bolstered by asset and lifecycle assessments, allowing operators to maintain grid reliability while minimizing downtime and service disruptions. On the side of the distribution/transformation, big data can support localized, customer-focused applications. Real-time sensing and asset management deliver detailed operational information, enabling efficient outage detection and restoration. Big data-based fault diagnosis, voltage and frequency control, and health monitoring/prediction improve the reliability and adaptability of distribution systems. In DSM, big data enables consumer-focused strategies to balance demand with available supply. Applications such as demand response management, load classification, and demand information systems provide actionable insights for both consumers and utilities. Tools, including customer load forecasting, energy-saving interactions, and protection/theft detection, enhance efficiency and security on the demand side. By utilizing these tools, DSM empowers consumers to actively participate in energy markets while supporting overall system stability.

Overall, big data and its analytics are the foundation and most important part of harnessing AI for the energy transition. In the following sections, LLMs and agentic AI strategies in power systems presented are fully dependent on big data.

Large language models in power systems

Large language models are advanced AI systems designed to process, understand, and generate human-like information by using vast amounts of data and advanced computational techniques (Chang et al., 2024; Naveed et al., 2025). Built on DL architecture, typically Transformer-based neural networks (Bouschery et al., 2023; Su et al., 2025), LLMs consist of vast amounts of parameters that enable them to capture intricate patterns. These models are trained on diverse datasets, including books, articles, websites, and other textual sources, allowing them to develop a broad knowledge base and the ability to perform different tasks. The training process involves unsupervised learning, where the model predicts the token in a sequence, and sometimes fine-tuning with supervised or Reinforcement Learning (RL) to align outputs with specific tasks. Power systems are also among these sectors in which LLMs can be used in different ways. As a case study of LLMs integration in the power systems, an example is manifested in Fig. 4.

The architecture of LLMs, in Fig. 4, is tied to the hardware they operate on, particularly in Transformer-based models running on a Personal Computer (PC) with Graphical Processing Unit (GPU) acceleration (Li, R et al., 2024; Koilia & Kachris, 2024). The computational pipeline starts with the Central Processing Unit (CPU) handling lightweight input processing by tokenizing text, followed by the transfer of tokenized data from Random Accessible Memory (RAM) to GPU memory through the Peripheral Component Interconnect Express (PCIe) bus (Saber & Jiang, 2025,

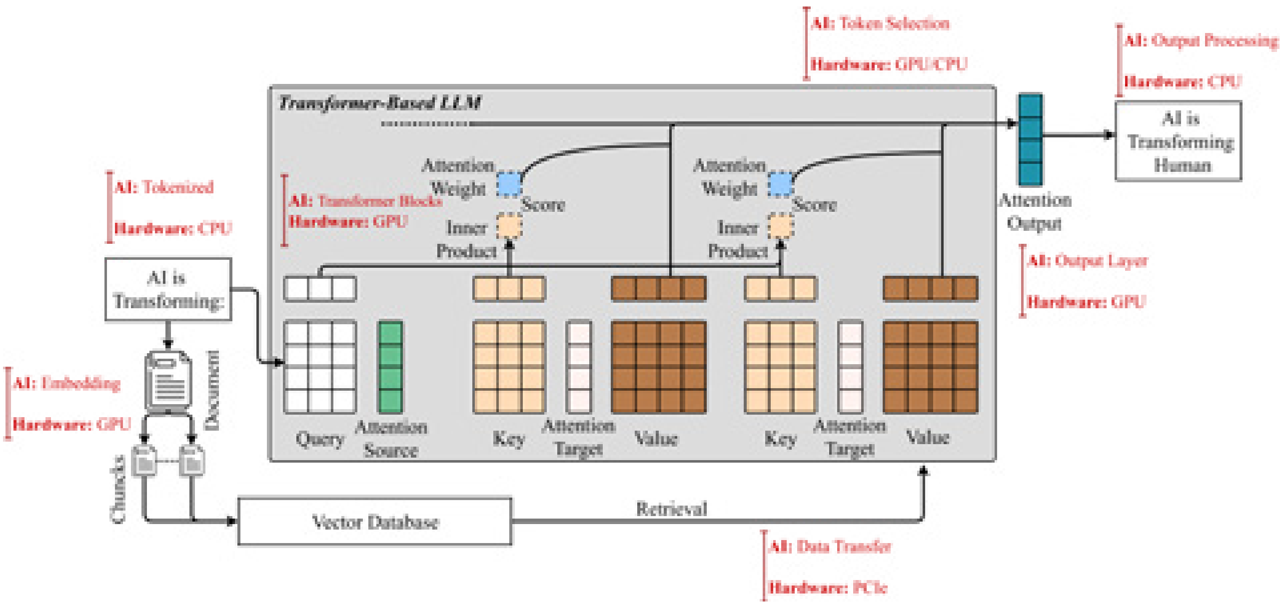

Figure 4: A case study of LLM integration in a power system, conceptualized from (Li, Y et al., 2024). This case study shows the LLM pipelines and the hardware process relationships.

Huang et al., 2025), which can become a challenge for large datasets. On the GPU, tokens are transformed into vector representations with positional encodings during the embedding phase, a task of moderate computational intensity. The core of the LLM's workload occurs in the Transformer blocks, where the GPU's parallel processing excels in executing multi-head self-attention, layer normalization, and Feed-Forward Neural Network (FFNN) operations, leading to the resource-intensive stage and highlighting the critical role of GPU acceleration. Subsequently, the GPU performs a final linear transformation and Softmax operation (Zimerman et al., 2024; Jha & Reagen, 2024; Rakka et al., 2025) in the output layer to generate token probabilities, after which token selection involves both GPU and CPU to choose the next token based on these probabilities. The CPU then converts the selected token back into text during output processing, with steps including data transfer, embedding, Transformer block computations, output layer processing, token selection, and output processing repeating iteratively for multi-token generation. The computational demands of LLMs scale with model size and hardware capabilities, which can run on mid-range GPUs, while larger models necessitate high-end or multiple GPUs. This interdependence presents the GPU's important effect on handling the extensive matrix operations within Transformer blocks, forming the computational foundation of modern LLMs (Li, Y et al., 2024), being used in different power system applications. Additionally, an overview of recent works presented LLMs integration in power systems is given in Table 1.

Table 1: Some of the works considered agentic AI strategies in power systems

Strategy	System	Insights	Ref.
Fine-Tuned LLM	Power System Load Profile	Fine-tuned LLMs to reduce data needs in power system load profile analysis by restoring missing data. It proposes a two-stage fine-tuning strategy, demonstrating that the fine-tuned model matches the performance of specialized models. Key insights emphasized the role of prompt engineering and few-shot learning for efficient knowledge transfer.	(Hu et al., 2025)
Pre-Trained LLM	Building	Black-box tuning inductive adapter based on pre-trained LLMs, designed for short-term building-level load forecasting to enhance power grid stability and efficiency. Addressing the challenge of limited or unavailable historical load data, it used LLMs' generalization capabilities without requiring domain-specific pre-training or fine-tuning. It considered spatial correlations among nearby buildings to improve forecast accuracy and adapt to varying building sizes.	(Zhou & Wang, 2025)
Prompting LLM	Wind Turbine	A hard-soft hybrid prompt learning method to enhance wind power forecasting (WPF) using an LLM, addressing two key challenges: inflexible forecasting horizons and prediction errors due to chaotic wind speed mutations under varying geographic and atmospheric conditions. A hard prompt generator redefines WPF as a language modeling task, leveraging the LLM's representation learning to capture temporal features and detect mutations in wind power data. A soft-prompt adapter with gated attention aligns the LLM to the WPF context through parameter-efficient tuning, capturing spatial-temporal characteristics across wind farms.	(Duan et al., 2025)
LLM-SUC	Wind Energy System	A hybrid method integrating LLMs with a multi-scenario stochastic unit commitment (SUC) framework to boost efficiency and reliability in power systems amid high wind uncertainties. In 10 trials, LLM-SUC cut average total costs by 1.1–2.7% ($185.58M vs. $187.68M for traditional SUC) and load curtailment by 26.3% (2.24 ± 0.31 GWh vs. 3.04 GWh), with zero wind curtailment.	(Ren et al., 2025)
LLM-DRL	Distribution Networks	A regional voltage control approach for distribution grids featuring extensive Distributed Energy Resources (DERs), tackling issues of voltage breaches and grid losses. It fuses Deep Reinforcement Learning (DRL) with LLM tools by prompt engineering to create tailored datasets for DRL agent training.	(Yan & Cheng, 2025)

Continue (Table 1)

Strategy	System	Insights	Ref.
Fine-Tuned LLM	Distribution Networks	A DL method employing a fine-tuned LLM to solve the distribution network reconfiguration challenge in power grids with DER and heightened customer involvement. Through engineered prompts and a bespoke loss function, the LLM learns from bus, line, voltage, and loss data to forecast optimal setups that reduce losses while satisfying operational limits.	(Christou et al., 2025)
LLMs	Smart Grids	Review of LLMs in power systems, evaluating 30 practical implementations in key areas: Grid Operations and Management, Energy Markets and Trading, Personalized Energy Management and Customer Engagement, Grid Planning and Education, Grid Security and Compliance, Advanced Data Analysis and Knowledge Discovery, Emerging Applications and Societal Impact, and LLM-Enhanced RL. By fusing live grid information, market fluctuations, and user patterns, LLMs facilitated dynamic operations, anticipatory protection, and tailored energy offerings. The analysis tackles hurdles in data privacy and model dependability, offering strategies for ethical and fair implementation.	(Madani et al., 2025)
LLM	Industrial Control System	A strategy merging data-driven and design-driven techniques to create attack sequences for assessing ML resilience in Industrial Control Systems (ICS) by LLMs. Countering issues of limited testing environments, expensive expert input, and sparse attack datasets, this approach employs LLMs to yield superior and more plentiful attack patterns compared to human-generated ones.	(Ahmed, 2025)
LLM-Multi-Task Learning	Integrated Energy Systems	A zero-shot forecasting model for energy loads powered by LLMs to handle growing complexity and variability in integrated energy setups incorporating renewables. The model features a preprocessing unit for multi-source load data, a prompt creation module employing multi-task learning and similarity matching to close semantic divides, and a forecasting unit leveraging pre-trained LLMs.	(Li et al., 2025)
LLM	Power System	An LLM-powered autonomous research system that applies a reflection-evolution technique to autonomously tackle intricate power system research problems without human oversight. It manages devices, collects data, devises approaches, and refines algorithms for tasks in parameter prediction, power optimization, and state estimation.	(Liu et al., 2025)
Multi-Agent-LLM-CGAN	EV Charging System	An EV charging platform employing multi-agent LLMs to streamline integration of EV charging with grid scheduling. It incorporates a user agent delivering customized charging advice from past records and a station agent that dynamically sets prices via fine-tuned LLMs, linked through a negotiation hub for protected data exchange. A Conditional Generative Adversarial Network (CGAN) produces synthetic user habits and pricing info to boost LLM refinement.	(Niu et al., 2025)
Feedback-Based Multi-Agent LLM	Power System Simulations	A feedback-guided, multi-agent architecture that combines LLMs with experimental tools to advance power system modeling, surmounting LLMs' gaps in specialized expertise, logical processing, and parameter management. The architecture comprises an upgraded Retrieval-Augmented Generation (RAG) component, a refined reasoning unit, and an adaptive interaction module featuring error-feedback mechanisms.	(Jia et al., 2025)

Continue (Table 1)

Strategy	System	Insights	Ref.
LLM	Power Grid Graph Embedding	A framework crafted to tackle Optimal Power Flow (OPF) challenges in power systems via LLMs. It merges graph-based and tabular depictions of grids to adeptly query LLMs, capturing intricate interdependencies and limits. The system applies customized in-context learning and fine-tuning methods for LLMs.	(Bernier et al., 2025)
LLM & Power AI	Urban Distribution Network	A system fusing an LLM with a versatile power AI engine to support interactive and dependable dispatching in city distribution grids. To overcome LLMs' weaknesses in precise numerical calculations and adherence to rigid power rules, it employs a dispatcher-tool structure for concurrent cooperation via formatted data exchanges. It further integrates stepwise chain-of-thought logic, rejection sampling, and guided fine-tuning to guarantee rule conformity and elevate effectiveness.	(Zhu et al., 2025)
Optimized LLM	Distribution Power Grid Insulators	A hybrid DL system for forecasting surges in leakage current on high-voltage insulators from surface pollutants, which may trigger discharges and system failures. The system integrates multi-objective tuning via tree-structured Parzen estimation, a noise-suppression input filter, and an LLM for sequential forecasting to track and curb fault escalation.	(Matos-Carvalho et al., 2025)
LLM	Power System Dispatch	An LLM presented to advance power dispatch processes by overcoming traditional approaches' shortcomings in managing the magnitude, intricacy, and multitasking needs of contemporary power grids. It aids in operational adjustments, oversight, and black start situations via an innovative dataset assembly method that merges varied data origins for fine-tuning, plus targeted prompt tactics to maximize input-output performance.	(Cheng et al., 2025)
LLM	Urban Power Grid	An LLM-based system for building a specialized lexicon in urban power grid engineering, countering issues of outdated terms, meaning vagueness, and narrow word scope in conventional approaches. It assembles a structured dataset from official and sector standards, applying an advanced Term Frequency–Inverse Document Frequency (TF-IDF) method incorporating mutual information and adjacency entropy to derive 3426 premium initial terms. Hierarchical prompt designs and LLM self-correction facilitate synonym extraction, yielding 10745 equivalents with a mean cosine similarity of 0.86 and 89.3% precision.	(Xu et al., 2025)

Following Table 1, LLMs' applications are increasing in power systems by addressing complex challenges across diverse aspects, including load forecasting, wind power prediction, grid optimization, and security. Through advanced strategies, such as fine-tuning, prompt engineering, and multi-agent frameworks, LLMs enhance forecasting accuracy, optimize resource allocation, and improve operational resilience in scenarios with limited data or high uncertainty. By integrating real-time data, using generalization capabilities, and supporting tasks of network reconfiguration and anomaly detection, LLMs enable scalable, efficient, and adaptive solutions, significantly advancing smart grid technologies, urban power systems, and renewable energy integration, which manifests LLMs' increasing importance. Consequently, the much-advanced form of LLMs, known as agentic AI, is considered in the next section, and its applications in power systems are taken into consideration.

Agentic artificial intelligence in power systems

Agentic AI refers to AI systems designed with a high degree of autonomy, decision-making capability, and goal-oriented behavior, enabling them to act independently in dynamic environments to achieve specific objectives (Acharya et al., 2025; Bandi et al., 2025). Unlike traditional AI, which often relies on

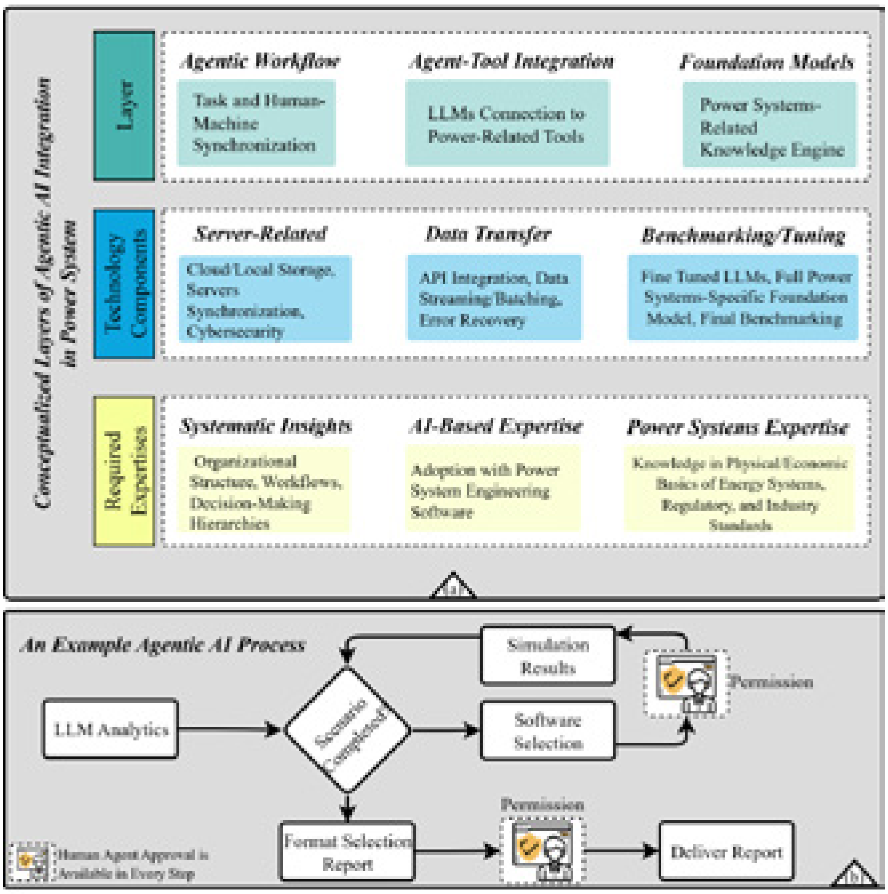

Figure 5: Agentic AI strategy for power systems: (1) Overall layers of its integration, and (b) Example utilized agentic AI, known as PowerAgent (Conceptualized from Zhang & Xie, 2025)

predefined rules or human oversight, agentic AI models use advanced techniques, such as RL (Zhang et al., 2025), LLMs, and contextual reasoning (Singh et al., 2025, Ren et al., 2025, Biswas & Talukdar, 2025), to perceive their surroundings, reason about complex scenarios, and execute actions with minimal human intervention. These systems are characterized by their ability to adapt to new information, learn from experience, and make decisions aligned with long-term goals, often in unpredictable or partially observable environments. An example of an agentic AI model, utilized for power systems, is shown in Fig. 5.

As the case study of agentic AI in power systems, the PowerAgent framework is presented (Zhang & Xie, 2025), built on three essential layers: (1) Foundation models that deliver broad intelligence capabilities, (2) Model Context Protocols (MCPs) that connect models with tools, and (3) Agentic workflows that facilitate real-world task execution through coordinated, modular AI behaviors. This modular structure enhances implementation clarity and aligns with evolving AI development trends, enabling the power sector to efficiently adapt and scale agentic intelligence. At the main center of PowerAgent lies a three-layered ecosystem comprising workflow automation, tool integration, and domain-specific foundation models (Fig. 5 (a)). These layers collectively provide a flexible and scalable foundation for agentic AI applications. The proposed agentic AI strategy, in Fig. 5 (b), integrates a domain-tailored LLM with MCPs and predefined workflows, enabling it to function as a virtual agent. When a user submits a query, such as evaluating potential power load demand growth in a specific region, the LLM processes the request and independently selects an appropriate analysis workflow. For instance, this workflow might include performing contingency analyses to assess how different load growth scenarios could impact transmission line congestion or voltage issues. Instead of directly resolving the query, the LLM uses MCP to interface with external tools, such as professional-grade simulation software, to handle technical computations. This separation of roles is advantageous in precision and reliability by using trusted industry-standard platforms. A defining feature of this agentic workflow is its adaptable human-in-the-loop approach. For sensitive tasks, including running simulations or altering system settings, the LLM may seek user approval before proceeding. For instance, after conducting scenario analyses, the LLM presents the results to the user for review and potential adjustments, keeping human oversight central to critical decisions. This approach is practical for security control applications where system safety requires careful monitoring (Zhang & Xie, 2025). Additionally, several other works, considered agentic AI strategies in power systems are presented in Table 2.

Table 2: Some of the works considered agentic AI strategies in power systems

Strategy	System	Insights	Ref.
Agentic AI-based Mathematical Framework	Electrical Distribution Systems	A dual-agent Proximal Policy Optimization (PPO) and market-based mechanisms to enhance electrical distribution system resilience against extreme weather and cyber threats. A strategic agent optimizes Distributed Energy Resources (DER)-driven configurations, while a tactical agent adjusts switch states under constraints.	(Johri et al., 2025)
Multi-Agentic AI	Built Environments	Review of agentic AI in built environments, proposing a classification framework for applications, functional roles, and learning approaches. It analyzed five key applications, categorized AI roles using the Data-Information-Knowledge-Wisdom (DIKW) hierarchy, and identified four learning approaches. Defining agentic built environments as AI-powered virtual assistants, it evaluated their development, limitations, and future directions for scalable, intelligent services across the building lifecycle.	(Lee et al., 2025)
Agentic AI (Copilot Models and Assistants)	Smart Systems	Review of agentic AI's potential in smart systems, highlighting its autonomy, reactivity, proactivity, and learning capabilities through different tools. It addresses the research gap in synthesizing agentic AI's diverse functionalities and a strategic framework for adopting generative AI, focusing on business needs, tool selection, and risk management. While Agentic AI boosts productivity, reduces costs, and drives innovation, challenges of privacy concerns persist.	(Hosseini & Seilani, 2025)
Agentic Digital Twin	Energy Sector	Review of the expanding role of AI, particularly Transformer models and LLMs, in enhancing energy management within smart grids. It reviewed the architectural foundations, domain-specific adaptations, and practical applications, highlighting generative AI's growing influence in high-level planning and daily operations of grid balancing and workforce training. It introduced the Agentic Digital Twin, a model integrating LLMs to enable autonomous, proactive, and socially interactive energy management systems.	(Antonesi et al., 2025)

The proposed advancements and recent works on agentic AI's application in power systems manifest the overall interest in it.

Challenges and future work

The integration of big data, Agentic AI, and LLMs is transforming power systems, including data centers, enabling real-time monitoring, predictive analytics, autonomous decision-making, and enhanced operator support. However, incorporating these technologies into critical infrastructure presents technical, operational, and regulatory challenges. To ensure safe, reliability, and sustainable deployment, the primary challenges (Fig. 6 (a)) should be identified and then associated with future research directions (Fig. 6 (b)) provided.

A. *Challenges*

The main challenges are presented in Fig. 6 (a).

The massive volume, high velocity, diverse formats, missing values, and limited labeled data complicate reliable analytics, while having data privacy, interoperability, and cybersecurity across complex pipelines remains a critical issue. Agentic AI, despite its potential for autonomous control, struggles with safety, explainability, and verification, especially when interacting with legacy systems and critical infrastructure, and coordinating multiple agents under partial observability, real-time constraints, and uncertain market incentives adds further complexity. LLMs face risks such as hallucinations, lack of operational grounding, limited domain knowledge, and integration challenges with real-time control, alongside high computational and energy demands that raise sustainability concerns. On the other hand, those AI technologies are heavily reliant on the data centers and their efficient performance, which increases the workload and the energy consumed. Meanwhile, data centers contend with power–thermal workload coupling, reliability–sustainability trade-offs, and unpredictable load behavior, all while needing to provide flexible demand response to support the grid.

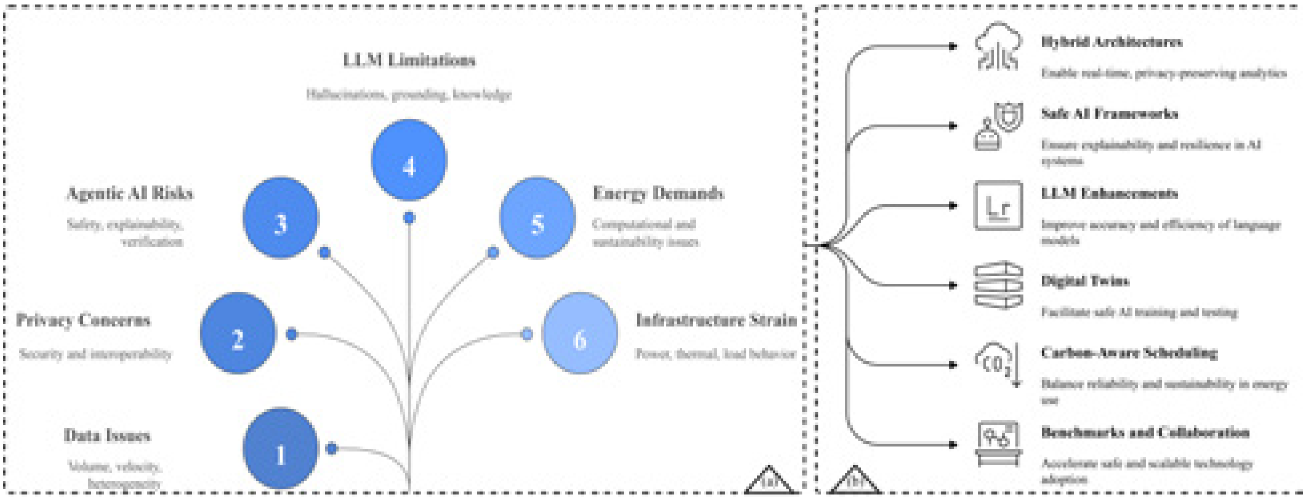

Figure 6: Big data, agentic AI, and LLMs integration in power systems: (a) Challenges, and (b) Associated future works (Source: Authors)

Figure 7: Proposed UN's SDGs related to the harnessing AI for energy transition

B. *Future works*

The future works associated with the presented challenges are shown in Fig. 6 (b). Future research should prioritize developing hybrid edge–cloud big data architectures, adaptive sampling, and more advanced self-supervised learning to enable real-time, privacy-preserving, and resource-efficient analytics. Safe and explainable agentic AI frameworks are essential, incorporating formal verification, human-in-the-loop oversight, and resilient multi-agent coordination for distributed systems, including microgrids and data centers. For LLMs, future research directions can focus on retrieval-augmented grounding, uncertainty quantification, domain-specific fine-tuning, and efficient model distillation for on-premises deployment. Cross-domain opportunities include creating digital twins of power systems and data centers for safe AI training and testing. Additionally, carbon-aware scheduling and co-optimisation of data-center workloads, facility thermal systems, and grid participation are among other strategies for balancing reliability and sustainability. Benchmarks are also helpful to further accelerate the safe, auditable, and scalable adoption of these technologies in the use of AI for energy transition.

C. *Alignment with UN-SDGs*

The UN's SDGs, adopted in 2015, are a set of seventeen interconnected global goals aimed at addressing pressing challenges, including poverty, inequality, climate change, and environmental degradation, by 2030. These goals provide a shared blueprint for governments, organizations, and individuals to promote prosperity, protect the planet, and ensure peace and justice for all (Carlsen & Bruggemann, 2022; Fernandes & Rodrigues, 2025). Among these seventeen SDGs, five of them are directly related to the use of AI in energy transition, shown in Fig. 7.

The integration of big data, agentic AI, and LLM is important in advancing SDG 7 (Pang & Chen, 2025, Zhao et al., 2025) (the most relevant SDG), which aims to ensure access to affordable, reliable, sustainable, and modern energy for all. Big data and AI optimize energy systems by enhancing grid efficiency, predicting energy demand, and facilitating the integration of renewable sources. Agentic AI can autonomously manage energy storage and distribution, ensuring stability in renewable-heavy grids. Meanwhile, LLMs can process wide datasets to recommend policies, technologies, or investment strategies for clean energy adoption. By enabling smarter energy management, reducing reliance on fossil fuels, and supporting the transition to sustainable energy systems, these technologies make energy more accessible and environmentally friendly, directly supporting the goals of SDG 7.

The SDG 9 focuses on building resilient infrastructure, promoting inclusive and sustainable industrialization, and advancing innovation (Aziz et al., 2025, Pauliukevičienė et al., 2025). Following this, the proposed AI technologies are impactful in achieving these objectives within the energy sector. Big data and AI drive advancements in energy infrastructure through innovations of smart grids, which enhance energy distribution, and predictive maintenance systems that ensure the reliability of renewable energy installations. LLMs accelerate research and development by analyzing large amounts of scientific literature and proposing novel energy solutions, such as advanced battery technologies or grid optimization techniques.

In the third relevant goal, SDG 11 aims to make cities inclusive, safe, resilient, and sustainable (Bleil de Souza et al., 2025, Wang et al., 2025), and the application of big data, agentic AI, and LLMs in the energy transition significantly contributes to this goal. AI-driven smart city solutions optimize energy use in urban settings, such as in buildings, public transportation, and street lighting, reducing energy waste and emissions. Big data analytics can identify urban energy consumption patterns, enabling targeted efficiency improvements. LLMs can support urban planners by analyzing data to design sustainable energy policies or simulate the impact of renewable energy integration in cities. Additionally, SDG 12 promotes sustainable consumption and production patterns in which big data, agentic AI, and LLMs are advantageous by optimizing resource use in the energy sector (Tsai et al., 2025; Cifuentes-Faura, 2025; Oliveira & Gomes, 2025; Precious, 2025). Big data and AI enhance efficiency in energy production by minimizing waste, optimizing supply chains, and improving the lifecycle management of energy infrastructure. Agentic AI can automate processes to ensure resources are used sustainably, such as prioritizing renewable energy in production systems. LLMs are also considered important by educating stakeholders on sustainable practices, analyzing supply chains for energy-efficient improvements, or generating reports to guide policy decisions.

Climate change is another critical issue that the whole world is now facing. In sequence, SDG 13 calls for urgent action to combat climate change, its impacts (Seddik & Sovacool, 2025, Zhang et al., 2025; Ji et al., 2025). To this end, the energy transition, powered by big data, agentic AI, and LLMs, can be a main solution to this effort. Big data analytics enable real-time monitoring of emissions, optimization of energy consumption, and prediction of climate-related impacts on energy systems. Agentic AI can autonomously implement carbon-neutral strategies, such as optimizing renewable energy deployment or managing carbon capture systems. LLMs can analyze climate data or help create public awareness campaigns to promote sustainable behaviors.

Conclusion

This article presented the significance of big data in power systems, alongside advanced AI approaches such as LLMs and agentic AI. For LLMs and agentic AI alike, a dedicated case study is examined for each, drawing on multiple recent literature and emerging advancements. Finally, the discussion addresses key challenges and prospective research avenues, enriched by descriptions of the UN-SDGs (7,9,11,12,13). Massive, high-velocity data with diverse formats, missing values, and scarce labels can cause challenges in analytics, alongside privacy, interoperability, and cybersecurity issues in complex pipelines. Agentic AI's autonomy is undermined by safety, explainability, and verification challenges, especially in larger systems, alongside the coordination under partial observability, real-time constraints, and uncertain incentives. LLMs sometimes have hallucinations, poor grounding, domain gaps, integration hurdles, and energy-intensive demands threatening sustainability. These technologies strain data centers facing power-thermal coupling, reliability-sustainability trade-offs, unpredictable loads, and grid demand response needs. Future work can focus on hybrid edge-cloud architectures, adaptive sampling, and self-supervised learning for real-time, private, efficient analytics. For LLMs, focus can be on retrieval-augmented grounding, uncertainty quantification, fine-tuning, and distillation for on-premises use. Safe, explainable agentic AI needs verification, human oversight, and multi-agent coordination for power systems. Cross-domain efforts include digital twins for safe AI training, as well as the carbon-aware scheduling and co-optimization of workloads, thermals, and grids for reliability and sustainability. Combined and developed, AI can have a considerably important role in the energy transition to a net-zero system, with near-zero reliance on fossil fuels, as a critical step towards combating climate change.

Ethical considerations

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